

Substance Name	CASRN	Lab	In Vitro Concentration Tested	In Vitro Physical Form Tested	Purity (%)	Solubility ^a	pH	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B) ^b	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score ^c	S-Score Classification	Overall S-Score Classification	Q-Score ^d	Q-Score Classification	Overall Q-Score Classification	IS(B)-10 ^e	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100 ^f	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Triethanolamine	102-71-6		10%	Solution	n.p.			10.75		Severe																Bagley et al. (1992)	
Triton X-100	9002-93-1		1%	Solution	n.p.			9		Severe																Bagley et al. (1992)	
Acetone	67-64-1	1	100%	Liquid	>99	water soluble												18.36	Severe	Severe							Balls et al. (1995)
Acetone	67-64-1	2	100%	Liquid	>99	water soluble												13.53	Severe								Balls et al. (1995)
Acetone	67-64-1	3	100%	Liquid	>99	water soluble												0.80	Nonirritant								Balls et al. (1995)
Acetone	67-64-1	4	100%	Liquid	>99	water soluble												10.31	Severe								Balls et al. (1995)
Ammonium nitrate	6484-52-2	1	100%	Solid	>99.9	water soluble												1.80	Moderate	Moderate							Balls et al. (1995)
Ammonium nitrate	6484-52-2	3	100%	Solid	>99.9	water soluble												1.30	Nonirritant								Balls et al. (1995)
Ammonium nitrate	6484-52-2	2	100%	Solid	>99.9	water soluble												18.00	Severe	Severe							Balls et al. (1995)
Ammonium nitrate	6484-52-2	4	100%	Solid	>99.9	water soluble												12.00	Moderate								Balls et al. (1995)
L-Aspartic acid	70-47-3	1	100%	Solid	95	water soluble												0.00	Nonirritant	Nonirritant							Balls et al. (1995)
L-Aspartic acid	70-47-3	2	100%	Solid	95	water soluble												1.00	Nonirritant	Moderate							Balls et al. (1995)
L-Aspartic acid	70-47-3	3	100%	Solid	95	water soluble												2.00	Nonirritant								Balls et al. (1995)
L-Aspartic acid	70-47-3	4	100%	Solid	95	water soluble												6.00	Moderate							Balls et al. (1995)	
Benzalkonium chloride	8001-54-5	1	1%	Solution	98	surfactant												3.41	Severe	Severe							Balls et al. (1995)
Benzalkonium chloride	8001-54-5	2	1%	Solution	98	surfactant												5.00	Severe								Balls et al. (1995)
Benzalkonium chloride	8001-54-5	3	1%	Solution	98	surfactant												3.90	Severe								Balls et al. (1995)
Benzalkonium chloride	8001-54-5	4	1%	Solution	98	surfactant												4.39	Severe								Balls et al. (1995)
Benzalkonium chloride	8001-54-5	1	5%	Solution	98	surfactant												6.93	Severe	Severe							Balls et al. (1995)
Benzalkonium chloride	8001-54-5	2	5%	Solution	98	surfactant												4.43	Severe								Balls et al. (1995)
Benzalkonium chloride	8001-54-5	3	5%	Solution	98	surfactant												1.20	Nonirritant								Balls et al. (1995)
Benzalkonium chloride	8001-54-5	4	5%	Solution	98	surfactant												6.49	Severe								Balls et al. (1995)
Benzalkonium chloride	8001-54-5	1	10%	Solution	98	surfactant												6.09	Severe	Severe							Balls et al. (1995)
Benzalkonium chloride	8001-54-5	2	10%	Solution	98	surfactant												7.03	Severe								Balls et al. (1995)
Benzalkonium chloride	8001-54-5	3	10%	Solution	98	surfactant												3.10	Severe								Balls et al. (1995)
Benzalkonium chloride	8001-54-5	4	10%	Solution	98	surfactant												6.14	Severe								Balls et al. (1995)

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Benzoyl-L-tartaric acid	2743-38-6	1	100%	Solid	n.p.	water soluble									0.00	Nonirritant										Balls et al. (1995)	
Benzoyl-L-tartaric acid	2743-38-6	3	100%	Solid	n.p.	water soluble									4.00	Nonirritant										Balls et al. (1995)	
Butyl acetate	123-86-4	1	100%	Liquid	99	water insoluble												1.55	Moderate								Balls et al. (1995)
Butyl acetate	123-86-4	2	100%	Liquid	99	water insoluble												1.23	Nonirritant								Balls et al. (1995)
Butyl acetate	123-86-4	3	100%	Liquid	99	water insoluble												1.80	Moderate								Balls et al. (1995)
Butyl acetate	123-86-4	4	100%	Liquid	99	water insoluble												1.93	Moderate								Balls et al. (1995)
Gamma-butyrolactone	96-48-0	1	100%	Liquid	>99	water soluble												22.04	Severe								Balls et al. (1995)
Gamma-butyrolactone	96-48-0	2	100%	Liquid	>99	water soluble												6.64	Severe								Balls et al. (1995)
Gamma-butyrolactone	96-48-0	3	100%	Liquid	>99	water soluble												1.97	Moderate								Balls et al. (1995)
Gamma-butyrolactone	96-48-0	4	100%	Liquid	>99	water soluble												4.02	Severe								Balls et al. (1995)
Captan 90 concentrate	133-06-2	1	100%	Solid	90	water soluble										0.00	Nonirritant									Balls et al. (1995)	
Captan 90 concentrate	133-06-2	3	100%	Solid	90	water soluble										0.00	Nonirritant									Balls et al. (1995)	
Captan 90 concentrate	133-06-2	4	100%	Solid	90	water soluble										6.00	Moderate									Balls et al. (1995)	
4-Carboxybenzaldehyde	619-66-9	1	100%	Solid	95	water insoluble										0.00	Nonirritant									Balls et al. (1995)	
4-Carboxybenzaldehyde	619-66-9	2	100%	Solid	95	water insoluble										6.00	Moderate									Balls et al. (1995)	
4-Carboxybenzaldehyde	619-66-9	3	100%	Solid	95	water insoluble										6.00	Moderate									Balls et al. (1995)	
4-Carboxybenzaldehyde	619-66-9	4	100%	Solid	95	water insoluble										4.00	Nonirritant									Balls et al. (1995)	
Cetylpyridinium bromide	140-72-7	1	0.10%	Solution	98	surfactant												2.43	Severe								Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	2	0.10%	Solution	98	surfactant												0.00	Nonirritant								Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	3	0.10%	Solution	98	surfactant												1.00	Nonirritant								Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	4	0.10%	Solution	98	surfactant												0.00	Nonirritant								Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	1	6%	Solution	98	surfactant												2.34	Severe								Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	2	6%	Solution	98	surfactant												2.42	Severe								Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	3	6%	Solution	98	surfactant												1.30	Nonirritant								Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	4	6%	Solution	98	surfactant												3.11	Severe								Balls et al. (1995)

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Cetylpyridinium bromide	140-72-7	1	10%	Solution	98	surfactant											2.71	Severe	Severe							Balls et al. (1995)		
Cetylpyridinium bromide	140-72-7	2	10%	Solution	98	surfactant											2.73	Severe								Balls et al. (1995)		
Cetylpyridinium bromide	140-72-7	3	10%	Solution	98	surfactant											1.80	Moderate								Balls et al. (1995)		
Cetylpyridinium bromide	140-72-7	4	10%	Solution	98	surfactant											4.67	Severe								Balls et al. (1995)		
Chlorhexidine	55-56-1	1	100%	Solid	99.5	water insoluble									3.00	Nonirritant	Moderate								Balls et al. (1995)			
Chlorhexidine	55-56-1	3	100%	Solid	99.5	water insoluble									6.00	Moderate									Balls et al. (1995)			
Chlorhexidine	55-56-1	4	100%	Solid	99.5	water insoluble									11.00	Moderate									Balls et al. (1995)			
Cyclohexanol	108-93-0	1	100%	Liquid	97	water soluble											3.28	Severe	Severe							Balls et al. (1995)		
Cyclohexanol	108-93-0	2	100%	Liquid	97	water soluble											4.48	Severe								Balls et al. (1995)		
Cyclohexanol	108-93-0	3	100%	Liquid	97	water soluble											5.20	Severe								Balls et al. (1995)		
Cyclohexanol	108-93-0	4	100%	Liquid	97	water soluble											6.69	Severe								Balls et al. (1995)		
Dibenzyl phosphate	1623-08-1	1	100%	Solid	99.5	water insoluble									0.00	Nonirritant	Severe								Balls et al. (1995)			
Dibenzyl phosphate	1623-08-1	2	100%	Solid	99.5	water insoluble									18.00	Severe									Balls et al. (1995)			
Dibenzyl phosphate	1623-08-1	3	100%	Solid	99.5	water insoluble									0.00	Nonirritant									Balls et al. (1995)			
Dibenzyl phosphate	1623-08-1	4	100%	Solid	99.5	water insoluble									15.00	Severe									Balls et al. (1995)			
2,6-Dichlorobenzoyl chloride	4659-45-4	1	100%	Liquid	99	water insoluble											10.14	Severe	Severe							Balls et al. (1995)		
2,6-Dichlorobenzoyl chloride	4659-45-4	2	100%	Liquid	99	water insoluble											8.81	Severe								Balls et al. (1995)		
2,6-Dichlorobenzoyl chloride	4659-45-4	3	100%	Liquid	99	water insoluble											1.90	Moderate								Balls et al. (1995)		
2,6-Dichlorobenzoyl chloride	4659-45-4	4	100%	Liquid	99	water insoluble											2.53	Severe								Balls et al. (1995)		
2,2-Dimethylbutanoic acid	595-37-9	1	100%	Liquid	>99	water insoluble											14.05	Severe	Severe							Balls et al. (1995)		
2,2-Dimethylbutanoic acid	595-37-9	2	100%	Liquid	>99	water insoluble											10.64	Severe								Balls et al. (1995)		
2,2-Dimethylbutanoic acid	595-37-9	3	100%	Liquid	>99	water insoluble											11.70	Severe								Balls et al. (1995)		
2,2-Dimethylbutanoic acid	595-37-9	4	100%	Liquid	>99	water insoluble											14.73	Severe								Balls et al. (1995)		
2,5-Dimethylhexanediol	110-03-2	1	100%	Solid	99.5	water insoluble											2.07	Severe	Severe							Balls et al. (1995)		
2,5-Dimethylhexanediol	110-03-2	3	100%	Solid	99.5	water insoluble											0.80	Nonirritant								Balls et al. (1995)		
2,5-Dimethylhexanediol	110-03-2	2	100%	Solid	99.5	water insoluble											18.00	Severe	Severe							Balls et al. (1995)		
2,5-Dimethylhexanediol	110-03-2	4	100%	Solid	99.5	water insoluble											18.00	Severe								Balls et al. (1995)		

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Ethanol	64-17-5	1	100%	Liquid	n.p.	water soluble												6.45	Severe	Severe							Balls et al. (1995)
Ethanol	64-17-5	2	100%	Liquid	n.p.	water soluble												10.63	Severe								Balls et al. (1995)
Ethanol	64-17-5	3	100%	Liquid	n.p.	water soluble												1.47	Nonirritant								Balls et al. (1995)
Ethanol	64-17-5	4	100%	Liquid	n.p.	water soluble												5.95	Severe								Balls et al. (1995)
Ethyl acetate	141-78-6	1	100%	Liquid	99	water soluble												3.94	Severe	Severe							Balls et al. (1995)
Ethyl acetate	141-78-6	2	100%	Liquid	99	water soluble												1.87	Moderate								Balls et al. (1995)
Ethyl acetate	141-78-6	3	100%	Liquid	99	water soluble												0.90	Nonirritant								Balls et al. (1995)
Ethyl acetate	141-78-6	4	100%	Liquid	99	water soluble												3.37	Severe								Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	1	100%	Liquid	99	water soluble												1.24	Nonirritant	Nonirritant							Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	2	100%	Liquid	99	water soluble												0.61	Nonirritant								Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	3	100%	Liquid	99	water soluble												1.00	Nonirritant								Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	4	100%	Liquid	99	water soluble												3.12	Severe								Balls et al. (1995)
Ethyl-2-methylacetacetate	609-14-3	1	100%	Liquid	ca. 97	water insoluble												2.40	Severe	Severe							Balls et al. (1995)
Ethyl-2-methylacetacetate	609-14-3	2	100%	Liquid	ca. 97	water insoluble												2.51	Severe								Balls et al. (1995)
Ethyl-2-methylacetacetate	609-14-3	3	100%	Liquid	ca. 97	water insoluble												1.10	Nonirritant								Balls et al. (1995)
Ethyl-2-methylacetacetate	609-14-3	4	100%	Liquid	ca. 97	water insoluble												2.35	Severe								Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	1	100%	Liquid	99	water insoluble												0.10	Nonirritant	Nonirritant							Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	2	100%	Liquid	99	water insoluble												0.19	Nonirritant								Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	3	100%	Liquid	99	water insoluble												0.30	Nonirritant								Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	4	100%	Liquid	99	water insoluble												1.01	Nonirritant								Balls et al. (1995)
Fomesafen	72128-02-0	1	100%	Solid	97.5	water soluble												0.00	Nonirritant	Moderate							Balls et al. (1995)
Fomesafen	72128-02-0	2	100%	Solid	97.5	water soluble												9.00	Moderate								Balls et al. (1995)
Fomesafen	72128-02-0	3	100%	Solid	97.5	water soluble												6.00	Moderate								Balls et al. (1995)
Fomesafen	72128-02-0	4	100%	Solid	97.5	water soluble												6.00	Moderate								Balls et al. (1995)

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Glycerol	56-81-5	1	100%	Liquid	99.5	water soluble												0.08	Nonirritant	Nonirritant							Balls et al. (1995)
Glycerol	56-81-5	2	100%	Liquid	99.5	water soluble												1.24	Nonirritant								Balls et al. (1995)
Glycerol	56-81-5	3	100%	Liquid	99.5	water soluble												0.60	Nonirritant								Balls et al. (1995)
Glycerol	56-81-5	4	100%	Liquid	99.5	water soluble												1.22	Nonirritant								Balls et al. (1995)
Hexanol	111-27-3	1	100%	Liquid	98	water insoluble												5.01	Severe	Severe							Balls et al. (1995)
Hexanol	111-27-3	2	100%	Liquid	98	water insoluble												3.98	Severe								Balls et al. (1995)
Hexanol	111-27-3	3	100%	Liquid	98	water insoluble												1.80	Moderate								Balls et al. (1995)
Hexanol	111-27-3	4	100%	Liquid	98	water insoluble												4.71	Severe								Balls et al. (1995)
Imidazole	288-32-4	1	100%	Solid	99	water soluble												11.19	Severe	Severe							Balls et al. (1995)
Imidazole	288-32-4	3	100%	Solid	99	water soluble												3.50	Severe								Balls et al. (1995)
Imidazole	288-32-4	2	100%	Solid	99	water soluble												18.00	Severe	Severe							Balls et al. (1995)
Imidazole	288-32-4	4	100%	Solid	99	water soluble												18.00	Severe								Balls et al. (1995)
Isobutanol	78-83-1	1	100%	Liquid	99.9	water insoluble												4.59	Severe	Severe							Balls et al. (1995)
Isobutanol	78-83-1	2	100%	Liquid	99.9	water insoluble												3.58	Severe								Balls et al. (1995)
Isobutanol	78-83-1	3	100%	Liquid	99.9	water insoluble												1.20	Nonirritant								Balls et al. (1995)
Isobutanol	78-83-1	4	100%	Liquid	99.9	water insoluble												5.89	Severe								Balls et al. (1995)
Isopropanol	67-63-0	1	100%	Liquid	99.9	water soluble												11.90	Severe	Severe							Balls et al. (1995)
Isopropanol	67-63-0	2	100%	Liquid	99.9	water soluble												5.79	Severe								Balls et al. (1995)
Isopropanol	67-63-0	3	100%	Liquid	99.9	water soluble												1.80	Moderate								Balls et al. (1995)
Isopropanol	67-63-0	4	100%	Liquid	99.9	water soluble												4.36	Severe								Balls et al. (1995)
Maneb	12427-38-2	1	100%	Solid	90	water soluble												0.00	Nonirritant	Nonirritant							Balls et al. (1995)
Maneb	12427-38-2	3	100%	Solid	90	water soluble												0.00	Nonirritant	Nonirritant							Balls et al. (1995)
Methyl acetate	79-20-9	1	100%	Liquid	98	water soluble												1.88	Moderate	Severe							Balls et al. (1995)
Methyl acetate	79-20-9	2	100%	Liquid	98	water soluble												5.39	Severe								Balls et al. (1995)
Methyl acetate	79-20-9	3	100%	Liquid	98	water soluble												1.70	Moderate								Balls et al. (1995)
Methyl acetate	79-20-9	4	100%	Liquid	98	water soluble												3.15	Severe								Balls et al. (1995)

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Methyl cyanoacetate	105-34-0	1	100%	Liquid	99	water soluble												1.51	Moderate	Moderate							Balls et al. (1995)
Methyl cyanoacetate	105-34-0	2	100%	Liquid	99	water soluble												1.21	Nonirritant								Balls et al. (1995)
Methyl cyanoacetate	105-34-0	3	100%	Liquid	99	water soluble												1.00	Nonirritant								Balls et al. (1995)
Methyl cyanoacetate	105-34-0	4	100%	Liquid	99	water soluble												1.78	Moderate								Balls et al. (1995)
Methylcyclopentane	96-37-7	1	100%	Liquid	>99	water insoluble												0.18	Nonirritant	Nonirritant							Balls et al. (1995)
Methylcyclopentane	96-37-7	2	100%	Liquid	>99	water insoluble												1.22	Nonirritant								Balls et al. (1995)
Methylcyclopentane	96-37-7	3	100%	Liquid	>99	water insoluble												0.20	Nonirritant								Balls et al. (1995)
Methylcyclopentane	96-37-7	4	100%	Liquid	>99	water insoluble												8.09	Severe								Balls et al. (1995)
Methyl ethyl ketone	78-93-3	1	100%	Liquid	99	water soluble												5.83	Severe	Severe							Balls et al. (1995)
Methyl ethyl ketone	78-93-3	2	100%	Liquid	99	water soluble												3.89	Severe								Balls et al. (1995)
Methyl ethyl ketone	78-93-3	3	100%	Liquid	99	water soluble												2.50	Severe								Balls et al. (1995)
Methyl ethyl ketone	78-93-3	4	100%	Liquid	99	water soluble												6.17	Severe								Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	1	100%	Liquid	98	water insoluble												2.29	Severe	Moderate							Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	2	100%	Liquid	98	water insoluble												1.04	Nonirritant								Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	3	100%	Liquid	98	water insoluble												1.50	Moderate								Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	4	100%	Liquid	98	water insoluble												1.86	Moderate								Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	1	100%	Solid	95	water soluble												3.84	Severe	Severe							Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	3	100%	Solid	95	water soluble												4.90	Severe								Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	2	100%	Solid	95	water soluble												18.00	Severe								Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	4	100%	Solid	95	water soluble												18.00	Severe								Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	1	100%	Solid	99	water soluble												6.00	Moderate	Moderate							Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	2	100%	Solid	99	water soluble												13.00	Moderate								Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	3	100%	Solid	99	water soluble												0.00	Nonirritant								Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	4	100%	Solid	99	water soluble												4.00	Nonirritant								Balls et al. (1995)

Substance Name	CASRN	Lab	In Vitro Concentration Tested	In Vitro Physical Form Tested	Purity (%)	Solubility*	pH	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	1S(B) [†]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score [‡]	S-Score Classification	Overall S-Score Classification	Q-Score [§]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10 [¶]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100 [¶]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Octanol	111-87-5	1	100%	Liquid	>99	water insoluble													2.10	Severe	Moderate						Balls et al. (1995)
Octanol	111-87-5	2	100%	Liquid	>99	water insoluble													1.00	Nonirritant							Balls et al. (1995)
Octanol	111-87-5	3	100%	Liquid	>99	water insoluble													1.80	Moderate							Balls et al. (1995)
Octanol	111-87-5	4	100%	Liquid	>99	water insoluble													1.78	Moderate							Balls et al. (1995)
Parafluoramine	371-40-4	1	100%	Liquid	99	water insoluble													5.25	Severe	Severe						Balls et al. (1995)
Parafluoramine	371-40-4	2	100%	Liquid	99	water insoluble													4.46	Severe							Balls et al. (1995)
Parafluoramine	371-40-4	3	100%	Liquid	99	water insoluble													1.90	Moderate							Balls et al. (1995)
Parafluoramine	371-40-4	4	100%	Liquid	99	water insoluble													2.57	Severe							Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	1	100%	Liquid	n.p.	surfactant													1.59	Moderate	Nonirritant						Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	2	100%	Liquid	n.p.	surfactant													0.72	Nonirritant							Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	3	100%	Liquid	n.p.	surfactant													0.60	Nonirritant							Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	4	100%	Liquid	n.p.	surfactant													1.22	Nonirritant							Balls et al. (1995)
Potassium cyanate	590-28-3	1	100%	Solid	97	water soluble													2.17	Severe	Severe						Balls et al. (1995)
Potassium cyanate	590-28-3	3	100%	Solid	97	water soluble													2.50	Severe							Balls et al. (1995)
Potassium cyanate	590-28-3	4	100%	Solid	97	water soluble													6.07	Severe							Balls et al. (1995)
Potassium cyanate	590-28-3	2	100%	Solid	97	water soluble													18.00	Severe	Severe						Balls et al. (1995)
Promethazine HCl	58-33-3	1	100%	Solid	98	water soluble													3.20	Severe	Severe						Balls et al. (1995)
Promethazine HCl	58-33-3	3	100%	Solid	98	water soluble													3.00	Severe							Balls et al. (1995)
Promethazine HCl	58-33-3	2	100%	Solid	98	water soluble													18.00	Severe							Balls et al. (1995)
Promethazine HCl	58-33-3	4	100%	Solid	98	water soluble													18.00	Severe							Balls et al. (1995)
Pyridine	110-86-1	1	100%	Liquid	>99	water soluble													3.84	Severe	Severe						Balls et al. (1995)
Pyridine	110-86-1	2	100%	Liquid	>99	water soluble													7.76	Severe							Balls et al. (1995)
Pyridine	110-86-1	3	100%	Liquid	>99	water soluble													12.90	Severe							Balls et al. (1995)
Pyridine	110-86-1	4	100%	Liquid	>99	water soluble													10.44	Severe							Balls et al. (1995)
Quinacrine	69-05-6	1	100%	Solid	n.p.	water soluble													0.00	Nonirritant	Nonirritant						Balls et al. (1995)
Quinacrine	69-05-6	3	100%	Solid	n.p.	water soluble													4.00	Nonirritant							Balls et al. (1995)
Quinacrine	69-05-6	4	100%	Solid	n.p.	water soluble													3.00	Nonirritant							Balls et al. (1995)

Substance Name	CASRN	Lab	In Vitro Conc. Tested	In Vitro Physical Form Tested	Purity (%)	Solubility*	pH	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	1S(B) ^j	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score ⁱ	Overall S-Score Classification	Q-Score ^j	Q-Score Classification	Overall Q-Score Classification	IS(B)-10 ^k	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100 ^k	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Sodium hydroxide	1310-73-2	1	1%	Solution	n.p.	water soluble									6.34	Severe	Severe								Balls et al. (1995)	
Sodium hydroxide	1310-73-2	2	1%	Solution	n.p.	water soluble									6.17	Severe									Balls et al. (1995)	
Sodium hydroxide	1310-73-2	3	1%	Solution	n.p.	water soluble									4.80	Severe									Balls et al. (1995)	
Sodium hydroxide	1310-73-2	4	1%	Solution	n.p.	water soluble									4.36	Severe									Balls et al. (1995)	
Sodium hydroxide	1310-73-2	1	10%	Solution	n.p.	water soluble									13.13	Severe	Severe								Balls et al. (1995)	
Sodium hydroxide	1310-73-2	2	10%	Solution	n.p.	water soluble									7.82	Severe									Balls et al. (1995)	
Sodium hydroxide	1310-73-2	3	10%	Solution	n.p.	water soluble									23.00	Severe									Balls et al. (1995)	
Sodium hydroxide	1310-73-2	4	10%	Solution	n.p.	water soluble									9.82	Severe									Balls et al. (1995)	
Sodium lauryl sulfate	151-21-3	1	3%	Solution	98	surfactant									2.68	Severe	Severe								Balls et al. (1995)	
Sodium lauryl sulfate	151-21-3	2	3%	Solution	98	surfactant									1.62	Moderate									Balls et al. (1995)	
Sodium lauryl sulfate	151-21-3	3	3%	Solution	98	surfactant									1.70	Moderate									Balls et al. (1995)	
Sodium lauryl sulfate	151-21-3	4	3%	Solution	98	surfactant									2.46	Severe									Balls et al. (1995)	
Sodium lauryl sulfate	151-21-3	1	15%	Solution	98	surfactant									2.86	Severe	Severe								Balls et al. (1995)	
Sodium lauryl sulfate	151-21-3	2	15%	Solution	98	surfactant									2.34	Severe									Balls et al. (1995)	
Sodium lauryl sulfate	151-21-3	3	15%	Solution	98	surfactant									1.80	Moderate									Balls et al. (1995)	
Sodium lauryl sulfate	151-21-3	4	15%	Solution	98	surfactant									4.37	Severe									Balls et al. (1995)	
Sodium oxalate	62-76-0	1	100%	Solid	>99	water soluble									0.00	Nonirritant	Moderate								Balls et al. (1995)	
Sodium oxalate	62-76-0	2	100%	Solid	>99	water soluble									12.00	Moderate									Balls et al. (1995)	
Sodium oxalate	62-76-0	3	100%	Solid	>99	water soluble									11.00	Moderate									Balls et al. (1995)	
Sodium oxalate	62-76-0	4	100%	Solid	>99	water soluble									9.00	Moderate									Balls et al. (1995)	
Sodium borate	10486-00-7	1	100%	Solid	98.6	water soluble									0.00	Nonirritant	Nonirritant								Balls et al. (1995)	
Sodium borate	10486-00-7	3	100%	Solid	98.6	water soluble									0.00	Nonirritant									Balls et al. (1995)	
Sodium borate	10486-00-7	4	100%	Solid	98.6	water soluble									7.00	Moderate									Balls et al. (1995)	
Tetraaminopyrimidine sulfate	5392-28-9	1	100%	Solid	97	water insoluble									0.00	Nonirritant	Nonirritant								Balls et al. (1995)	
Tetraaminopyrimidine sulfate	5392-28-9	3	100%	Solid	97	water insoluble									0.00	Nonirritant									Balls et al. (1995)	
Tetraaminopyrimidine sulfate	5392-28-9	4	100%	Solid	97	water insoluble									6.00	Moderate									Balls et al. (1995)	

Substance Name	CASRN	Lab	In Vitro Conc. Tested	In Vitro Physical Form Tested	Purity (%)	Solubility*	pH	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B) [†]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score [‡]	S-Score Classification	Overall S-Score Classification	Q-Score [§]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10 [¶]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100 [¶]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Thiourea	62-56-6	1	100%	Solid	>99	water soluble											1.31	Nonirritant	Nonirritant							Balls et al. (1995)	
Thiourea	62-56-6	3	100%	Solid	>99	water soluble											0.50	Nonirritant								Balls et al. (1995)	
Thiourea	62-56-6	2	100%	Solid	>99	water soluble									18.00	Severe	Severe								Balls et al. (1995)		
Thiourea	62-56-6	4	100%	Solid	>99	water soluble									13.00	Moderate									Balls et al. (1995)		
Toluene	108-88-3	1	100%	Liquid	99	water soluble											3.18	Severe	Severe							Balls et al. (1995)	
Toluene	108-88-3	2	100%	Liquid	99	water soluble											5.84	Severe								Balls et al. (1995)	
Toluene	108-88-3	3	100%	Liquid	99	water soluble											2.90	Severe								Balls et al. (1995)	
Toluene	108-88-3	4	100%	Liquid	99	water soluble											2.98	Severe								Balls et al. (1995)	
Trichloroacetic acid	76-03-9	1	3%	Solution	n.p.	water soluble											18.76	Severe	Severe							Balls et al. (1995)	
Trichloroacetic acid	76-03-9	2	3%	Solution	n.p.	water soluble											9.15	Severe								Balls et al. (1995)	
Trichloroacetic acid	76-03-9	3	3%	Solution	n.p.	water soluble											9.90	Severe								Balls et al. (1995)	
Trichloroacetic acid	76-03-9	4	3%	Solution	n.p.	water soluble											5.33	Severe								Balls et al. (1995)	
Trichloroacetic acid	76-03-9	1	30%	Solution	n.p.	water soluble											14.39	Severe	Severe							Balls et al. (1995)	
Trichloroacetic acid	76-03-9	2	30%	Solution	n.p.	water soluble											9.96	Severe								Balls et al. (1995)	
Trichloroacetic acid	76-03-9	3	30%	Solution	n.p.	water soluble											13.10	Severe								Balls et al. (1995)	
Trichloroacetic acid	76-03-9	4	30%	Solution	n.p.	water soluble											11.81	Severe								Balls et al. (1995)	
Triton X-100	9002-93-1	1	5%	Solution	98	surfactant											2.66	Severe	Severe							Balls et al. (1995)	
Triton X-100	9002-93-1	2	5%	Solution	98	surfactant											2.72	Severe								Balls et al. (1995)	
Triton X-100	9002-93-1	3	5%	Solution	98	surfactant											1.40	Nonirritant								Balls et al. (1995)	
Triton X-100	9002-93-1	4	5%	Solution	98	surfactant											2.20	Severe								Balls et al. (1995)	
Triton X-100	9002-93-1	1	10%	Solution	98	surfactant											3.45	Severe	Severe							Balls et al. (1995)	
Triton X-100	9002-93-1	2	10%	Solution	98	surfactant											1.71	Moderate								Balls et al. (1995)	
Triton X-100	9002-93-1	3	10%	Solution	98	surfactant											1.70	Moderate								Balls et al. (1995)	
Triton X-100	9002-93-1	4	10%	Solution	98	surfactant											2.40	Severe								Balls et al. (1995)	

Substance Name	CASRN	Lab	In Vitro Conc. Tested	In Vitro Physical Form Tested	Purity (%)	Solubility*	pH	IS(A)	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	1S(B) ^j	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score ⁱ	S-Score Classification	Overall S-Score Classification	Q-Score ^j	Q-Score Classification	Overall Q-Score Classification	IS(B)-10 ⁱ	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-10 ^j	IS(B)-100 ⁱ	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Tween 20	9005-64-5	1	100%	Liquid	98	surfactant										0.39	Nonirritant									Balls et al. (1995)			
Tween 20	9005-64-5	2	100%	Liquid	98	surfactant										0.38	Nonirritant									Balls et al. (1995)			
Tween 20	9005-64-5	3	100%	Liquid	98	surfactant										0.60	Nonirritant									Balls et al. (1995)			
Tween 20	9005-64-5	4	100%	Liquid	98	surfactant										0.95	Nonirritant									Balls et al. (1995)			
Acetic acid	64-19-7	2	100%	Liquid	>99						14.8															CEC (1991)			
Acetic acid	64-19-7	3	100%	Liquid	>99						13.7															CEC (1991)			
Acetic acid	64-19-7	4	100%	Liquid	>99						9.3															CEC (1991)			
Acetic acid	64-19-7	2	10%	Solution	>99						20.2															CEC (1991)			
Acetic acid	64-19-7	3	10%	Solution	>99						13.6															CEC (1991)			
Acetic acid	64-19-7	4	10%	Solution	>99						10.2															CEC (1991)			
Benzalkonium chloride	8001-54-5	2	100%	Unknown	n.p.						14.5															CEC (1991)			
Benzalkonium chloride	8001-54-5	3	100%	Unknown	n.p.						13.1															CEC (1991)			
Benzalkonium chloride	8001-54-5	5	100%	Unknown	n.p.						5.8															CEC (1991)			
Benzalkonium chloride	8001-54-5	6	100%	Unknown	n.p.						6.9															CEC (1991)			
Benzalkonium chloride	8001-54-5	7	100%	Unknown	n.p.						13.3															CEC (1991)			
Brij 35	9002-92-0	1	100%	Solid	>99						2.3															CEC (1991)			
Brij 35	9002-92-0	2	100%	Solid	>99						4.3															CEC (1991)			
Brij 35	9002-92-0	3	100%	Solid	>99						12.9															CEC (1991)			
Brij 35	9002-92-0	4	100%	Solid	>99						4.4															CEC (1991)			
Brij 35	9002-92-0	5	100%	Solid	>99						3.8															CEC (1991)			
Brij 35	9002-92-0	6	100%	Solid	>99						2.6															CEC (1991)			
Brij 35	9002-92-0	7	100%	Solid	>99						4															CEC (1991)			
Butanol	71-36-3	1	100%	Liquid	99						11.7															CEC (1991)			
Butanol	71-36-3	2	100%	Liquid	99						11.8															CEC (1991)			
Butanol	71-36-3	3	100%	Liquid	99						12.6															CEC (1991)			
Butanol	71-36-3	4	100%	Liquid	99						11.2															CEC (1991)			
Butanol	71-36-3	5	100%	Liquid	99						3.9															CEC (1991)			
Butanol	71-36-3	6	100%	Liquid	99						10.7															CEC (1991)			
Butanol	71-36-3	7	100%	Liquid	99						9.9															CEC (1991)			
Butanol	71-36-3	2	10%	Solution	99						14.2															CEC (1991)			

Substance Name	CASRN	Lab	In Vitro Concentration Tested	In Vitro Physical Form Tested	Purity (%)	Solubility ^a	pH	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B) ^j	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score ⁱ	S-Score Classification	Overall S-Score Classification	Q-Score ^k	Q-Score Classification	Overall Q-Score Classification	IS(B)-10 ^l	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100 ^m	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Butanol	71-36-3	3	10%	Solution	99						4.8		Slight	Severe												CEC (1991)	
Butanol	71-36-3	4	10%	Solution	99						12.5		Severe													CEC (1991)	
2-Butoxyethyl acetate	112-07-2	1	100%	Liquid	99						4.6		Slight													CEC (1991)	
2-Butoxyethyl acetate	112-07-2	2	100%	Liquid	99						5.3		Moderate													CEC (1991)	
2-Butoxyethyl acetate	112-07-2	3	100%	Liquid	99						4.7		Slight													CEC (1991)	
2-Butoxyethyl acetate	112-07-2	4	100%	Liquid	99						4.7		Slight													CEC (1991)	
2-Butoxyethyl acetate	112-07-2	5	100%	Liquid	99						4		Slight													CEC (1991)	
2-Butoxyethyl acetate	112-07-2	6	100%	Liquid	99						3.9		Slight													CEC (1991)	
2-Butoxyethyl acetate	112-07-2	7	100%	Liquid	99						4.5		Slight													CEC (1991)	
2-Butoxyethyl acetate	112-07-2	2	10%	Solution	99						4.1		Slight													CEC (1991)	
2-Butoxyethyl acetate	112-07-2	3	10%	Solution	99						0		Nonirritant													CEC (1991)	
2-Butoxyethyl acetate	112-07-2	4	10%	Solution	99						3.2		Slight													CEC (1991)	
Dibutyltin chloride	683-18-1	1	100%	Solid	97						11.6		Severe													CEC (1991)	
Dibutyltin chloride	683-18-1	2	100%	Solid	97						10.8		Severe													CEC (1991)	
Dibutyltin chloride	683-18-1	4	100%	Solid	97						12.6		Severe													CEC (1991)	
Dibutyltin chloride	683-18-1	5	100%	Solid	97						5.1		Moderate													CEC (1991)	
Dibutyltin chloride	683-18-1	6	100%	Solid	97						5		Moderate													CEC (1991)	
Dibutyltin chloride	683-18-1	7	100%	Solid	97						13		Severe													CEC (1991)	
Dimethyl sulfoxide	67-68-5	1	100%	Liquid	99.9						11.7		Severe													CEC (1991)	
Dimethyl sulfoxide	67-68-5	2	100%	Liquid	99.9						10.9		Severe													CEC (1991)	
Dimethyl sulfoxide	67-68-5	3	100%	Liquid	99.9						11.3		Severe													CEC (1991)	
Dimethyl sulfoxide	67-68-5	4	100%	Liquid	99.9						4.1		Slight													CEC (1991)	
Dimethyl sulfoxide	67-68-5	5	100%	Liquid	99.9						4.9		Slight													CEC (1991)	
Dimethyl sulfoxide	67-68-5	6	100%	Liquid	99.9						7.3		Moderate													CEC (1991)	
Dimethyl sulfoxide	67-68-5	7	100%	Liquid	99.9						11.4		Severe													CEC (1991)	

Substance Name	CASRN	Lab	In Vitro Conc. Tested	In Vitro Physical Form Tested	Purity (%)	Solubility ^a	pH	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B) ^b	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score ^c	S-Score Classification	Overall S-Score Classification	Q-Score ^d	Q-Score Classification	Overall Q-Score Classification	IS(B)-10 ^e	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100 ^f	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Dimethyl sulfoxide	67-68-5	2	10%	Solution	99.9						4.4		Slight	Slight											CEC (1991)		
Dimethyl sulfoxide	67-68-5	3	10%	Solution	99.9						4.1		Slight												CEC (1991)		
Dimethyl sulfoxide	67-68-5	4	10%	Solution	99.9						4.1		Slight												CEC (1991)		
Glycerol	56-81-5	1	100%	Liquid	>99						10.8		Severe	Severe											CEC (1991)		
Glycerol	56-81-5	2	100%	Liquid	>99						11.3		Severe												CEC (1991)		
Glycerol	56-81-5	3	100%	Liquid	>99						10.3		Severe												CEC (1991)		
Glycerol	56-81-5	4	100%	Liquid	>99						4.8		Slight												CEC (1991)		
Glycerol	56-81-5	5	100%	Liquid	>99						0		Nonirritant												CEC (1991)		
Glycerol	56-81-5	6	100%	Liquid	>99						0		Nonirritant												CEC (1991)		
Glycerol	56-81-5	7	100%	Liquid	>99						9.4		Severe												CEC (1991)		
Glycerol	56-81-5	2	10%	Solution	>99						8.7		Moderate	Slight											CEC (1991)		
Glycerol	56-81-5	3	10%	Solution	>99						4.4		Slight												CEC (1991)		
Glycerol	56-81-5	4	10%	Solution	>99						3.6		Slight												CEC (1991)		
n-Hexane	110-54-3	1	100%	Liquid	99						2.9		Slight	Slight											CEC (1991)		
n-Hexane	110-54-3	2	100%	Liquid	99						5.4		Moderate												CEC (1991)		
n-Hexane	110-54-3	3	100%	Liquid	99						4.2		Slight												CEC (1991)		
n-Hexane	110-54-3	4	100%	Liquid	99						10.3		Severe												CEC (1991)		
n-Hexane	110-54-3	5	100%	Liquid	99						2.3		Slight												CEC (1991)		
n-Hexane	110-54-3	6	100%	Liquid	99						8.1		Moderate												CEC (1991)		
n-Hexane	110-54-3	7	100%	Liquid	99						2.4		Slight												CEC (1991)		
n-Hexane	110-54-3	2	10%	Solution	99						3.7		Slight	Severe											CEC (1991)		
n-Hexane	110-54-3	3	10%	Solution	99						0		Nonirritant												CEC (1991)		
n-Hexane	110-54-3	4	10%	Solution	99						10.1		Severe												CEC (1991)		

Substance Name	CASRN	Lab	In Vitro Conc. Tested	In Vitro Physical Form Tested	Purity (%)	Solubility ^a	pH	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B) ^j	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score ⁱ	S-Score Classification	Overall S-Score Classification	Q-Score ^k	Q-Score Classification	Overall Q-Score Classification	IS(B)-10 ^l	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100 ^m	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
2-Methoxyethanol	109-86-4	1	100%	Liquid	99						9.7		Severe	Severe											CEC (1991)		
2-Methoxyethanol	109-86-4	2	100%	Liquid	99						12.2		Severe												CEC (1991)		
2-Methoxyethanol	109-86-4	3	100%	Liquid	99						12.1		Severe												CEC (1991)		
2-Methoxyethanol	109-86-4	4	100%	Liquid	99						8.6		Moderate												CEC (1991)		
2-Methoxyethanol	109-86-4	5	100%	Liquid	99						4.5		Slight												CEC (1991)		
2-Methoxyethanol	109-86-4	6	100%	Liquid	99						0.8		Nonirritant												CEC (1991)		
2-Methoxyethanol	109-86-4	7	100%	Liquid	99						3.1		Slight												CEC (1991)		
2-Methoxyethanol	109-86-4	2	10%	Solution	99						7		Moderate	Moderate											CEC (1991)		
2-Methoxyethanol	109-86-4	3	10%	Solution	99						0		Nonirritant													CEC (1991)	
2-Methoxyethanol	109-86-4	4	10%	Solution	99						3.1		Slight													CEC (1991)	
Sodium lauryl sulfate	151-21-3	1	100%	Solid	98						11.4		Severe	Severe												CEC (1991)	
Sodium lauryl sulfate	151-21-3	2	100%	Solid	98						10.3		Severe													CEC (1991)	
Sodium lauryl sulfate	151-21-3	3	100%	Solid	98						13.9		Severe													CEC (1991)	
Sodium lauryl sulfate	151-21-3	4	100%	Solid	98						4.8		Slight													CEC (1991)	
Sodium lauryl sulfate	151-21-3	6	100%	Solid	98						11.1		Severe													CEC (1991)	
Sodium lauryl sulfate	151-21-3	7	100%	Solid	98						9.7		Severe													CEC (1991)	
Sodium lauryl sulfate	151-21-3	2	10%	Solution	98						18.4		Severe	Severe												CEC (1991)	
Sodium lauryl sulfate	151-21-3	3	10%	Solution	98						14.1		Severe													CEC (1991)	
Sodium lauryl sulfate	151-21-3	4	10%	Solution	98						5.1		Moderate													CEC (1991)	
Toluene	108-88-3	1	100%	Liquid	99.9						8.8		Moderate	Severe												CEC (1991)	
Toluene	108-88-3	2	100%	Liquid	99.9						14.8		Severe													CEC (1991)	
Toluene	108-88-3	3	100%	Liquid	99.9						15.2		Severe													CEC (1991)	
Toluene	108-88-3	4	100%	Liquid	99.9						11.5		Severe													CEC (1991)	
Toluene	108-88-3	5	100%	Liquid	99.9						4.6		Slight													CEC (1991)	
Toluene	108-88-3	6	100%	Liquid	99.9						3.1		Slight													CEC (1991)	
Toluene	108-88-3	7	100%	Liquid	99.9						4.9		Slight													CEC (1991)	

Substance Name	CASRN	Lab	In Vitro Conc. Tested	In Vitro Physical Form Tested	Purity (%)	Solubility ^a	pH	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B) ^j	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score ⁱ	S-Score Classification	Overall S-Score Classification	Q-Score ^k	Q-Score Classification	Overall Q-Score Classification	IS(B)-10 ^l	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100 ^m	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Triacetin	102-76-1	1	100%	Liquid	99						3.6		Slight	Slight											CEC (1991)		
Triacetin	102-76-1	2	100%	Liquid	99						4.3		Slight												CEC (1991)		
Triacetin	102-76-1	3	100%	Liquid	99						5.5		Moderate												CEC (1991)		
Triacetin	102-76-1	4	100%	Liquid	99						4.4		Slight												CEC (1991)		
Triacetin	102-76-1	5	100%	Liquid	99						3.3		Slight												CEC (1991)		
Triacetin	102-76-1	6	100%	Liquid	99						4.3		Slight												CEC (1991)		
Triacetin	102-76-1	7	100%	Liquid	99						3.1		Slight												CEC (1991)		
Triacetin	102-76-1	2	10%	Solution	99						13.6		Severe	Slight											CEC (1991)		
Triacetin	102-76-1	3	10%	Solution	99						2		Slight												CEC (1991)		
Triacetin	102-76-1	4	10%	Solution	99						3.3		Slight												CEC (1991)		
Tributyltin chloride	1461-22-9	1	100%	Solid	96						6.7		Moderate	Moderate											CEC (1991)		
Tributyltin chloride	1461-22-9	2	100%	Solid	96						8.9		Moderate												CEC (1991)		
Tributyltin chloride	1461-22-9	3	100%	Solid	96						13.7		Severe												CEC (1991)		
Tributyltin chloride	1461-22-9	4	100%	Solid	96						8.8		Moderate												CEC (1991)		
Tributyltin chloride	1461-22-9	5	100%	Solid	96						7.4		Moderate												CEC (1991)		
Tributyltin chloride	1461-22-9	6	100%	Solid	96						7.9		Moderate												CEC (1991)		
Tributyltin chloride	1461-22-9	7	100%	Solid	96						6.6		Moderate												CEC (1991)		
Tributyltin chloride	1461-22-9	2	10%	Solution	96						15.6		Severe	Severe											CEC (1991)		
Tributyltin chloride	1461-22-9	3	10%	Solution	96						9.6		Severe												CEC (1991)		
Tributyltin chloride	1461-22-9	4	10%	Solution	96						11.2		Severe												CEC (1991)		
Triethanolamine	102-71-6	1	100%	Liquid	97						8.6		Moderate	Severe											CEC (1991)		
Triethanolamine	102-71-6	2	100%	Liquid	97						10.4		Severe												CEC (1991)		
Triethanolamine	102-71-6	3	100%	Liquid	97						11.9		Severe												CEC (1991)		
Triethanolamine	102-71-6	4	100%	Liquid	97						4.2		Slight												CEC (1991)		
Triethanolamine	102-71-6	5	100%	Liquid	97						0		Nonirritant												CEC (1991)		
Triethanolamine	102-71-6	6	100%	Liquid	97						3.7		Slight												CEC (1991)		
Triethanolamine	102-71-6	7	100%	Liquid	97						7.5		Moderate												CEC (1991)		

Substance Name	CASRN	Lab	In Vitro Conc. Tested	In Vitro Physical Form Tested	Purity (%)	Solubility ^a	pH	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B) ^j	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score ⁱ	S-Score Classification	Overall S-Score Classification	Q-Score ^k	Q-Score Classification	Overall Q-Score Classification	IS(B)-10 ^l	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100 ^m	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Triethanolamine	102-71-6	2	10%	Solution	97						11.3		Severe	Slight											CEC (1991)		
Triethanolamine	102-71-6	3	10%	Solution	97						2.8		Slight												CEC (1991)		
Triethanolamine	102-71-6	4	10%	Solution	97						1.1		Slight												CEC (1991)		
Hydroalcoholic Formulation 1-5% Alcohol Containing Formulation (PROD-00187)			100%	Solution	n.a.						4.6		Slight													Gettings et al. (1991)	
Hydroalcoholic Formulation 2-10% Alcohol Containing Formulation (PROD-00183)			100%	Solution	n.a.						5		Moderate													Gettings et al. (1991)	
Hydroalcoholic Formulation 3-15% Alcohol Containing Formulation (PROD-00186)			100%	Solution	n.a.						8.5		Moderate													Gettings et al. (1991)	
Hydroalcoholic Formulation 4-20% Alcohol Containing Formulation (PROD-00185)			100%	Solution	n.a.						5.3		Moderate													Gettings et al. (1991)	
Hydroalcoholic Formulation 5-33% Alcohol Containing Formulation (PROD-00184)			100%	Solution	n.a.																					Gettings et al. (1991)	
Hydroalcoholic Formulation 6-40% Alcohol Containing Formulation (PROD-00189)			100%	Solution	n.a.						11.9		Severe													Gettings et al. (1991)	
Hydroalcoholic Formulation 7-55% Alcohol Containing Formulation (PROD-00188)			100%	Solution	n.a.						12.8		Severe													Gettings et al. (1991)	
Hydroalcoholic Formulation 8-65% Alcohol Containing Formulation (PROD-00180)			100%	Solution	n.a.						12.7		Severe													Gettings et al. (1991)	
Hydroalcoholic Formulation 9-83% Alcohol Containing Formulation (PROD-00181)			100%	Solution	n.a.						13.8		Severe													Gettings et al. (1991)	
Hydroalcoholic Formulation 10-90% Alcohol Containing Formulation (PROD-00182)			100%	Solution	n.a.						13.6		Severe													Gettings et al. (1991)	
Oil/Water Emulsion-HZA			100%	Solution	n.a.		0		Nonirritant	Nonirritant	1		Slight													Gettings et al. (1994)	
Oil/Water Emulsion-HZC			100%	Solution	n.a.		0.283		Nonirritant	Nonirritant	3		Slight													Gettings et al. (1994)	
Oil/Water Emulsion-HZE			100%	Solution	n.a.		0.533		Nonirritant	Nonirritant	3.67		Slight													Gettings et al. (1994)	
Oil/Water Emulsion-HZF			100%	Solution	n.a.		7.33		Moderate	Moderate	3.67		Slight													Gettings et al. (1994)	

Substance Name	CASRN	Lab	In Vitro Conc. Tested	In Vitro Physical Form Tested	Purity (%)	Solubility ^a	pH	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B) ^b	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score ^c	S-Score Classification	Overall S-Score Classification	Q-Score ^d	Q-Score Classification	Overall Q-Score Classification	IS(B)-10 ^e	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100 ^f	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Oil/Water Emulsion-HZH ^g			100%	Solution	n.a.			17.8		Severe	Severe	23		Severe												Gettings et al. (1994)	
Oil/Water Emulsion-HZI			100%	Solution	n.a.			1.97		Slight	Slight	0.333		Nonirritant												Gettings et al. (1994)	
Oil/Water Emulsion-HZJ			100%	Solution	n.a.			0.917		Nonirritant	Nonirritant	3		Slight												Gettings et al. (1994)	
Oil/Water Emulsion-HZL			100%	Solution	n.a.			4.83		Slight	Slight	10.3		Severe												Gettings et al. (1994)	
Oil/Water Emulsion-HZM			100%	Solution	n.a.			8.33		Moderate	Moderate	14.3		Severe												Gettings et al. (1994)	
Oil/Water Emulsion-HZN			100%	Solution	n.a.			3.33		Slight	Slight	3.67		Slight											Gettings et al. (1994)		
Oil/Water Emulsion-HZO			100%	Solution	n.a.			0.5		Nonirritant	Nonirritant	0		Nonirritant											Gettings et al. (1994)		
Oil/Water Emulsion-HZR			100%	Solution	n.a.			10.6		Severe	Severe	16.3		Severe												Gettings et al. (1994)	
Oil/Water Emulsion-HZS			100%	Solution	n.a.			11.6		Severe	Severe	8.33		Moderate												Gettings et al. (1994)	
Oil/Water Emulsion-HZT			100%	Solution	n.a.			4.1		Slight	Slight	1		Slight												Gettings et al. (1994)	
Oil/Water Emulsion-HZU			100%	Solution	n.a.			0		Nonirritant	Nonirritant	1		Slight											Gettings et al. (1994)		
Oil/Water Emulsion-HZV			100%	Solution	n.a.			0.6		Nonirritant	Nonirritant	0		Nonirritant											Gettings et al. (1994)		
Oil/Water Emulsion-HZW			100%	Solution	n.a.			0.167		Nonirritant	Nonirritant	5		Moderate											Gettings et al. (1994)		
Oil/Water Emulsion-HZY			100%	Solution	n.a.			17		Severe	Severe	9.67		Severe											Gettings et al. (1994)		
Surfactant Based Formulation 1-HZA			10%	Solution	n.a.			7.8		Moderate	Moderate	9.6		Severe											Gettings et al. (1996)		
Surfactant Based Formulation 2-HZB			10%	Solution	n.a.			4.8		Slight	Slight	7.3		Moderate											Gettings et al. (1996)		
Surfactant Based Formulation 3-HZC			10%	Solution	n.a.			9.5		Severe	Severe	15.3		Severe											Gettings et al. (1996)		
Surfactant Based Formulation 4-HZD			10%	Solution	n.a.			5.2		Moderate	Moderate	8.7		Moderate											Gettings et al. (1996)		
Surfactant Based Formulation 5-HZE			10%	Solution	n.a.			3.8		Slight	Slight	11.4		Severe											Gettings et al. (1996)		
Surfactant Based Formulation 6-HZF			10%	Solution	n.a.			8.3		Moderate	Moderate	10.9		Severe											Gettings et al. (1996)		
Surfactant Based Formulation 7-HZG			10%	Solution	n.a.			6.3		Moderate	Moderate	7.1		Moderate											Gettings et al. (1996)		
Surfactant Based Formulation 8-HZH			10%	Solution	n.a.			1.3		Slight	Slight	3.5		Slight											Gettings et al. (1996)		
Surfactant Based Formulation 9-HZI			10%	Solution	n.a.			9.3		Severe	Severe	15.2		Severe											Gettings et al. (1996)		
Surfactant Based Formulation 10-HZJ			10%	Solution	n.a.			2.2		Slight	Slight	6.2		Moderate											Gettings et al. (1996)		
Surfactant Based Formulation 11-HZK			10%	Solution	n.a.			8.8		Moderate	Moderate	9.4		Severe											Gettings et al. (1996)		
Surfactant Based Formulation 12-HZL			10%	Solution	n.a.			9.6		Severe	Severe	12.4		Severe											Gettings et al. (1996)		
Surfactant Based Formulation 13-HZM			10%	Solution	n.a.			4.1		Slight	Slight	2.7		Slight											Gettings et al. (1996)		

Substance Name	CASRN	Lab	In Vitro Conc. Tested	In Vitro Physical Form Tested	Purity (%)	Solubility ^a	pH	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score ^c	S-Score Classification	Overall S-Score Classification	Q-Score ^d	Q-Score Classification	Overall Q-Score Classification	IS(B)-10 ^e	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100 ^f	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Surfactant Based Formulation 14-HZN			10%	Solution	n.a.			6.1	Moderate	Moderate	8	Moderate													Gettings et al. (1996)	
Surfactant Based Formulation 15-HZP			10%	Solution	n.a.			4.7	Slight	Slight	4.4	Slight													Gettings et al. (1996)	
Surfactant Based Formulation 16-HZQ			10%	Solution	n.a.			4.9	Slight	Slight	4.2	Slight													Gettings et al. (1996)	
Surfactant Based Formulation 17-HZR			10%	Solution	n.a.			7.7	Moderate	Moderate	5.3	Moderate													Gettings et al. (1996)	
Surfactant Based Formulation 18-HZS			10%	Solution	n.a.			8.8	Moderate	Moderate	12.2	Severe													Gettings et al. (1996)	
Surfactant Based Formulation 19-HZT			10%	Solution	n.a.			0.2	Nonirritant	Nonirritant	3.5	Slight													Gettings et al. (1996)	
Surfactant Based Formulation 20-HZU			10%	Solution	n.a.			3.7	Slight	Slight	6.2	Moderate													Gettings et al. (1996)	
Surfactant Based Formulation 21-HZV			10%	Solution	n.a.			7.7	Moderate	Moderate	8.7	Moderate													Gettings et al. (1996)	
Surfactant Based Formulation 22-HZW			10%	Solution	n.a.			7.8	Moderate	Moderate	5.1	Moderate													Gettings et al. (1996)	
Surfactant Based Formulation 23-HZX			10%	Solution	n.a.			9	Severe	Severe	11.3	Severe													Gettings et al. (1996)	
Surfactant Based Formulation 24-HZY			10%	Solution	n.a.			8.7	Moderate	Moderate	11.7	Severe													Gettings et al. (1996)	
Surfactant Based Formulation 25-HZZ			10%	Solution	n.a.			0.7	Nonirritant	Nonirritant	1.1	Slight													Gettings et al. (1996)	
Allyl alcohol	107-18-6		100%	Liquid	n.p.						12.4	2.3	Severe													Gilleron et al. (1996)
2-Aminophenol	95-55-6		100%	Solid	n.p.						0.8	0.7	Nonirritant													Gilleron et al. (1996)
Anthracene	120-12-7		100%	Solid	n.p.						0	0	Nonirritant													Gilleron et al. (1996)
Benzethonium chloride	121-54-0		100%	Solid	n.p.						15.4	3.1	Severe													Gilleron et al. (1996)
Gamma-butyrolactone	96-48-0		100%	Liquid	n.p.						13.9	1.8	Severe													Gilleron et al. (1996)
Cyclohexanone	108-94-1		100%	Liquid	n.p.						14.5	3.8	Severe													Gilleron et al. (1996)
Deoxycholic acid, sodium salt	302-95-4		100%	Solid	n.p.						9.7	5.8	Severe													Gilleron et al. (1996)
Diacetone alcohol	123-42-2		100%	Liquid	n.p.						15.1	2.7	Severe													Gilleron et al. (1996)
Dibenzoyl-L-tartaric acid	2743-38-6		100%	Solid	n.p.						4.2	2.5	Slight													Gilleron et al. (1996)
2,4-Dichloro-5-sulfamolybenzoic acid	2736-23-4		100%	Solid	n.p.						3.8	2.2	Slight													Gilleron et al. (1996)
Dimethyl biguanidine	657-24-9		100%	Solid	n.p.						8.4	2.2	Moderate													Gilleron et al. (1996)
Dimethyl sulfoxide	67-68-5		100%	Liquid	n.p.						11.3	3.7	Severe													Gilleron et al. (1996)
EDTA dipotassium	25105-12-9		100%	Solid	n.p.						0	0	Nonirritant													Gilleron et al. (1996)
Ethanol	64-17-5		100%	Liquid	n.p.						11.3	2.8	Severe													Gilleron et al. (1996)
2-Ethoxyethanol	110-80-5		100%	Liquid	n.p.						10.5	2.7	Severe													Gilleron et al. (1996)

Substance Name	CASRN	Lab	In Vitro Conc. Tested	In Vitro Physical Form Tested	Purity (%)	Solubility ^a	pH	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B) ^b SD	IS(B) Classification	Overall IS(B) Classification	S-Score ^c	S-Score Classification	Overall S-Score Classification	Q-Score ^d	Q-Score Classification	Overall Q-Score Classification	IS(B)-10 ^e	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100 ^f	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Ethylacetacetate	141-97-9		100%	Liquid	n.p.						10	3.2	Severe												Gilleron et al. (1996)	
Furan	110-00-9		100%	Liquid	n.p.						5.5	1	Moderate												Gilleron et al. (1996)	
Glucosolactone	90-80-2		100%	Solid	n.p.						4.6	3.2	Slight												Gilleron et al. (1996)	
DL-Glutamic acid	19285-83-7		100%	Solid	n.p.						0.7	1.2	Nonirritant												Gilleron et al. (1996)	
3-Glycidopropyltrimethoxysilane	2530-83-8		100%	Liquid	n.p.						4.3	1	Slight												Gilleron et al. (1996)	
Hexadecyltrimethylammonium bromide	57-09-0		100%	Liquid	n.p.						10.8	4.8	Severe												Gilleron et al. (1996)	
Hexane	110-54-3		100%	Liquid	n.p.						3.1	2.7	Slight												Gilleron et al. (1996)	
Imidazole	288-32-4		100%	Solid	n.p.						18.7	0.9	Severe												Gilleron et al. (1996)	
Iminodibenzyl	94-19-9		100%	Solid	n.p.						0	0	Nonirritant												Gilleron et al. (1996)	
N-Lauroylsarcosine, sodium salt	7631-98-3		100%	Solid	n.p.						12.7	4.3	Severe												Gilleron et al. (1996)	
Laurylsulfobetaine	14933-08-5		100%	Unknown	n.p.						8.3	1.2	Moderate												Gilleron et al. (1996)	
Magnesium carbonate	56378-72-4		100%	Solid	n.p.						1.4	1.9	Slight												Gilleron et al. (1996)	
Methanol	67-56-1		100%	Liquid	n.p.						12.2	3.3	Severe												Gilleron et al. (1996)	
2-Methoxyethanol	109-86-4		100%	Liquid	n.p.						14.5	0.7	Severe												Gilleron et al. (1996)	
Methyl isobutyl ketone	108-10-1		100%	Liquid	n.p.						10.5	1.5	Severe												Gilleron et al. (1996)	
MYRJ 45			100%	Unknown	n.p.						0.00	0.00	Nonirritant												Gilleron et al. (1996)	
1-Nitropropane	108-03-2		100%	Liquid	n.p.						2.8	2.7	Slight												Gilleron et al. (1996)	
Octanol	111-87-5		100%	Liquid	n.p.						9.8	1.7	Severe												Gilleron et al. (1996)	
2,4-Pentadione	123-54-6		100%	Liquid	n.p.						8.8	3	Moderate												Gilleron et al. (1996)	
1-Phenyl-3-pyrazolidine	92-43-3		100%	Solid	n.p.						0.5	0.4	Nonirritant												Gilleron et al. (1996)	
Polyoxyethylene 23 lauryl ether			100%	Solid	n.p.						1.5	2.6	Slight												Gilleron et al. (1996)	
Promethazine HCl	58-33-3		100%	Solid	n.p.						13.9	2.1	Severe												Gilleron et al. (1996)	
Propyl-4-hydroxybenzoate	94-13-3		100%	Solid	n.p.						1.9	1	Slight												Gilleron et al. (1996)	
Pyridine	110-86-1		100%	Liquid	n.p.						15.8	3.6	Severe												Gilleron et al. (1996)	
Quinacrine	69-05-6		100%	Solid	n.p.						6.5	2.2	Moderate												Gilleron et al. (1996)	
Tetraaminopyrimidine sulfate	5392-28-9		100%	Solid	n.p.						0.5	0.9	Nonirritant												Gilleron et al. (1996)	
Thiourea	62-56-6		100%	Solid	n.p.						13.7	4.4	Severe												Gilleron et al. (1996)	

Substance Name	CASRN	Lab	In Vitro Conc. Tested	In Vitro Physical Form Tested	Purity (%)	Solubility ^a	pH	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B) ^j	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score ⁱ	S-Score Classification	Overall S-Score Classification	Q-Score ^k	Q-Score Classification	Overall Q-Score Classification	IS(B)-10 ^l	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100 ^m	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
1,2,3-Trichloropropane	96-18-4		100%	Liquid	n.p.						7.9	1.7	Moderate													Gilleron et al. (1996)	
1,2,4-Trichloropropane	95-63-6		100%	Liquid	n.p.						4.5	2.9	Slight													Gilleron et al. (1996)	
Triethanolamine	102-71-6		100%	Liquid	n.p.						9.6	3.5	Severe													Gilleron et al. (1996)	
Triton X-155	9010-44-0		100%	Surfactant	n.p.						3.9	2.3	Slight													Gilleron et al. (1996)	
Acetone	67-64-1		100%	Liquid	>99	water soluble					15.32	0.33	Severe													Gilleron et al. (1997)	
Ammonium nitrate	6484-52-2		100%	Solid	>99.9	water soluble					15.34	1.24	Severe													Gilleron et al. (1997)	
L-Aspartic acid	70-47-3		100%	Solid	95	water soluble					1.06	1.2	Slight													Gilleron et al. (1997)	
Benzalkonium chloride	8001-54-5		100%	Unknown	98	surfactant					14.8	0.53	Severe													Gilleron et al. (1997)	
Benzalkonium chloride	8001-54-5		100%	Unknown	98	surfactant					15.05	0.27	Severe													Gilleron et al. (1997)	
Benzalkonium chloride	8001-54-5		100%	Unknown	98	surfactant					15.14	0.25	Severe													Gilleron et al. (1997)	
Benzoyl-L-tartaric acid	2743-38-6		100%	Solid	n.p.	water soluble					13.34	4.24	Severe													Gilleron et al. (1997)	
Butyl acetate	123-86-4		100%	Liquid	99	water insoluble					17.21	1.84	Severe													Gilleron et al. (1997)	
Gamma-butyrolactone	96-48-0		100%	Liquid	>99	water soluble					19.39	0.83	Severe													Gilleron et al. (1997)	
Captan 90 concentrate	133-06-2		100%	Solid	90	water soluble					15.07	0.27	Severe													Gilleron et al. (1997)	
4-Carboxybenzaldehyde	619-66-9		100%	Solid	95	water insoluble					3.95	4.69	Slight													Gilleron et al. (1997)	
Cetylpyridinium bromide	140-72-7		100%	Solid	98	surfactant					12.68	1.52	Severe													Gilleron et al. (1997)	
Cetylpyridinium bromide	140-72-7		100%	Solid	98	surfactant					13.53	2.42	Severe													Gilleron et al. (1997)	
Cetylpyridinium bromide	140-72-7		100%	Solid	98	surfactant					14.6	0.43	Severe													Gilleron et al. (1997)	
Chlorhexidine	55-56-1		100%	Solid	99.5	water insoluble					14.87	3.78	Severe													Gilleron et al. (1997)	
Cyclohexanol	108-93-0		100%	Liquid	97	water soluble					18.96	0.1	Severe													Gilleron et al. (1997)	
Dibenzyl phosphate	1623-08-1		100%	Solid	99.5	water insoluble					15.16	0.47	Severe													Gilleron et al. (1997)	
2,6-Dichlorobenzoyl chlorid	4659-45-4		100%	Liquid	99	water insoluble					10.74	1.74	Severe													Gilleron et al. (1997)	
2,2-Dimethylbutanoic acid	595-37-9		100%	Liquid	>99	water insoluble					15.31	0.24	Severe													Gilleron et al. (1997)	
2,5-Dimethylhexanediol	110-03-2		100%	Solid	99.5	water insoluble					15.33	0.38	Severe													Gilleron et al. (1997)	
Ethanol	64-17-5		100%	Liquid	n.p.	water soluble					14.97	0.04	Severe													Gilleron et al. (1997)	
Ethyl acetate	141-78-6		100%	Liquid	99	water soluble					19.32	0.06	Severe													Gilleron et al. (1997)	
2-Ethyl-1-hexanol	104-76-7		100%	Liquid	99	water soluble					12.71	2.96	Severe													Gilleron et al. (1997)	

Substance Name	CASRN	Lab	In Vitro Conc. Tested	In Vitro Physical Form Tested	Purity (%)	Solubility*	pH	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score ¹	S-Score Classification	Overall S-Score Classification	Q-Score ¹	Q-Score Classification	Overall Q-Score Classification	IS(B)-10 ¹	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100 ¹	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Ethyl-2-methylacetooacetate	609-14-3		100%	Liquid	ca. 97	water insoluble				12.94	2.94	Severe													Gilleron et al. (1997)	
Ethyl trimethyl acetate	3938-95-2		100%	Liquid	99	water insoluble				13.82	2.73	Severe													Gilleron et al. (1997)	
Fomesafen	72128-02-0		100%	Solid	97.5	water soluble				1.21	1.29	Slight													Gilleron et al. (1997)	
Glycerol	56-81-5		100%	Liquid	99.5	water soluble				14.78	0.75	Severe													Gilleron et al. (1997)	
Hexanol	111-27-3		100%	Liquid	98	water insoluble				17.56	0.4	Severe													Gilleron et al. (1997)	
Imidazole	288-32-4		100%	Solid	99	water soluble				19.43	0.49	Severe													Gilleron et al. (1997)	
Isobutanol	78-83-1		100%	Liquid	99.9	water insoluble				19.41	0.08	Severe													Gilleron et al. (1997)	
Isopropanol	67-63-0		100%	Liquid	99.9	water soluble				14.8	0.21	Severe													Gilleron et al. (1997)	
Maneb	12427-38-2		100%	Solid	90	water soluble				0.16	0.24	Nonirritant													Gilleron et al. (1997)	
Methyl acetate	79-20-9		100%	Liquid	98	water soluble				18.98	0.75	Severe													Gilleron et al. (1997)	
Methyl cyanoacetate	105-34-0		100%	Liquid	99	water soluble				16.31	1.23	Severe													Gilleron et al. (1997)	
Methylcyclopentane	96-37-7		100%	Liquid	>99	water insoluble				17.14	1.63	Severe													Gilleron et al. (1997)	
Methyl ethyl ketone	78-93-3		100%	Liquid	99	water soluble				18.35	2.52	Severe													Gilleron et al. (1997)	
Methyl isobutyl ketone	108-10-1		100%	Liquid	98	water insoluble				17.75	2.2	Severe													Gilleron et al. (1997)	
1-Naphthalene acetic acid	86-87-3		100%	Solid	99	water soluble				7.46	2.37	Moderate													Gilleron et al. (1997)	
1-Naphthalene acetic acid, Na salt	61-31-4		100%	Solid	95	water soluble				15.16	0.49	Severe													Gilleron et al. (1997)	
Octanol	111-87-5		100%	Liquid	>99	water insoluble				16.7	0.81	Severe													Gilleron et al. (1997)	
Parahoraniline	371-40-4		100%	Liquid	99	water insoluble				15.49	1.63	Severe													Gilleron et al. (1997)	
Polyethylene glycol 400	25322-68-3		100%	Liquid	n.p.	surfactant				14.68	0.55	Severe													Gilleron et al. (1997)	
Potassium cyanate	590-28-3		100%	Solid	97	water soluble				14.27	1.15	Severe													Gilleron et al. (1997)	
Promethazine HCl	58-33-3		100%	Solid	98	water soluble				6.27	1.41	Moderate													Gilleron et al. (1997)	
Pyridine	110-86-1		100%	Liquid	>99	water soluble				17.79	2.44	Severe													Gilleron et al. (1997)	
Quinacrine	69-05-6		100%	Solid	n.p.	water soluble				7.29	0.6	Moderate													Gilleron et al. (1997)	
Sodium hydroxide	1310-73-2		100%	Solid	n.p.	water soluble				19.01	0.13	Severe													Gilleron et al. (1997)	
Sodium hydroxide	1310-73-2		100%	Solid	n.p.	water soluble				20.56	0.08	Severe													Gilleron et al. (1997)	
Sodium lauryl sulfate	151-21-3		100%	Solid	98	surfactant				12.38	1.82	Severe													Gilleron et al. (1997)	
Sodium lauryl sulfate	151-21-3		100%	Solid	98	surfactant				15.05	0.29	Severe													Gilleron et al. (1997)	

Substance Name	CASRN	Lab	In Vitro Conc. Tested	In Vitro Physical Form Tested	Purity (%)	Solubility*	pH	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B) ^j	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score ⁱ	S-Score Classification	Overall S-Score Classification	Q-Score ^k	Q-Score Classification	Overall Q-Score Classification	IS(B)-10 ^l	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-10 ^l	IS(B)-100 ^l	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Sodium oxalate	62-76-0		100%	Solid	>99	water soluble					14.2	0.71	Severe													Gilleron et al. (1997)		
Sodium perborate	10486-00-7		100%	Solid	98.6	water soluble					13.19	1.78	Severe													Gilleron et al. (1997)		
Tetraaminopyrimidine sulfate	5392-28-9		100%	Solid	97	water insoluble					4.33	0.23	Slight													Gilleron et al. (1997)		
Thiourea	62-56-6		100%	Solid	>99	water soluble					17.89	1.53	Severe													Gilleron et al. (1997)		
Toluene	108-88-3		100%	Liquid	99	water soluble					16.09	1.62	Severe													Gilleron et al. (1997)		
Trichloroacetic acid	76-03-9		100%	Liquid	n.p.	water soluble					15.7	0.11	Severe													Gilleron et al. (1997)		
Trichloroacetic acid	76-03-9		100%	Liquid	n.p.	water soluble					15.72	0.15	Severe													Gilleron et al. (1997)		
Triton X-100	9002-93-1		100%	Liquid	98	surfactant					10.94	0.8	Severe													Gilleron et al. (1997)		
Triton X-100	9002-93-1		100%	Liquid	98	surfactant					13.73	0.48	Severe													Gilleron et al. (1997)		
Tween 20	9005-64-5		100%	Liquid	98	surfactant					14.47	0.36	Severe													Gilleron et al. (1997)		
Acetic acid	64-19-7	1	10%	Solution	n.p.		2.4	16.5	2.89	Severe	Severe														Hagino et al. (1999) Submitted Y. Ohno Data			
Acetic acid	64-19-7	2	10%	Solution	n.p.		2.4	16	3.92	Severe															Hagino et al. (1999) Submitted Y. Ohno Data			
Acetic acid	64-19-7	3	10%	Solution	n.p.		2.4	17.25	6.24	Severe															Hagino et al. (1999) Submitted Y. Ohno Data			
Acetic acid	64-19-7	4	10%	Solution	n.p.		2.4	19.5	1.91	Severe															Hagino et al. (1999) Submitted Y. Ohno Data			
Acetic acid	64-19-7	5	10%	Solution	n.p.		2.4	17.5	4.04	Severe															Hagino et al. (1999) Submitted Y. Ohno Data			
Butanol	71-36-3	1	10%	Suspension	n.p.		7.31	8.25	2.87	Moderate	Severe														Hagino et al. (1999) Submitted Y. Ohno Data			
Butanol	71-36-3	2	10%	Suspension	n.p.		7.31	10.5	1.91	Severe															Hagino et al. (1999) Submitted Y. Ohno Data			
Butanol	71-36-3	3	10%	Suspension	n.p.		7.31	12	0.00	Severe															Hagino et al. (1999) Submitted Y. Ohno Data			
Butanol	71-36-3	4	10%	Suspension	n.p.		7.31	12	0.00	Severe															Hagino et al. (1999) Submitted Y. Ohno Data			
Butanol	71-36-3	5	10%	Suspension	n.p.		7.31	5.75	1.50	Moderate															Hagino et al. (1999) Submitted Y. Ohno Data			

Substance Name	CASRN	Lab	In Vitro Conc. Tested	In Vitro Physical Form Tested	Purity (%)	Solubility*	pH	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B) ^j	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score ⁱ	Overall S-Score Classification	Q-Score ^j	Q-Score Classification	Overall Q-Score Classification	IS(B)-10 ⁱ	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100 ⁱ	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Cetyltrimethylammonium bromide	57-09-0	1	10%	Solution	n.p.		5.89	19	1.63	Severe	Severe														Hagino et al. (1999) Submitted Y. Ohio Data	
Cetyltrimethylammonium bromide	57-09-0	2	10%	Solution	n.p.		5.89	13.25	2.22	Severe															Hagino et al. (1999) Submitted Y. Ohio Data	
Cetyltrimethylammonium bromide	57-09-0	3	10%	Solution	n.p.		5.89	18.5	1.91	Severe															Hagino et al. (1999) Submitted Y. Ohio Data	
Cetyltrimethylammonium bromide	57-09-0	4	10%	Solution	n.p.		5.89	11	2.45	Severe															Hagino et al. (1999) Submitted Y. Ohio Data	
Cetyltrimethylammonium bromide	57-09-0	5	10%	Solution	n.p.		5.89	9	0.00	Severe															Hagino et al. (1999) Submitted Y. Ohio Data	
Chlorhexidine gluconate solution (20% solution)	18472-51-0	1	10%	Solution	n.p.		6.56	19	1.63	Severe	Severe														Hagino et al. (1999) Submitted Y. Ohio Data	
Chlorhexidine gluconate solution (20% solution)	18472-51-0	2	10%	Solution	n.p.		6.56	13.5	1.00	Severe															Hagino et al. (1999) Submitted Y. Ohio Data	
Chlorhexidine gluconate solution (20% solution)	18472-51-0	3	10%	Solution	n.p.		6.56	16	2.45	Severe															Hagino et al. (1999) Submitted Y. Ohio Data	
Chlorhexidine gluconate solution (20% solution)	18472-51-0	4	10%	Solution	n.p.		6.56	11.75	4.86	Severe															Hagino et al. (1999) Submitted Y. Ohio Data	
Chlorhexidine gluconate solution (20% solution)	18472-51-0	5	10%	Solution	n.p.		6.56	9	0.00	Severe															Hagino et al. (1999) Submitted Y. Ohio Data	
Di(2-ethylhexyl) sodium sulfosuccinate	577-11-7	1	10%	Suspension	n.p.		6.54	10	0.00	Severe	Severe														Hagino et al. (1999) Submitted Y. Ohio Data	
Di(2-ethylhexyl) sodium sulfosuccinate	577-11-7	2	10%	Suspension	n.p.		6.54	10	1.63	Severe															Hagino et al. (1999) Submitted Y. Ohio Data	
Di(2-ethylhexyl) sodium sulfosuccinate	577-11-7	3	10%	Suspension	n.p.		6.54	10.25	3.50	Severe															Hagino et al. (1999) Submitted Y. Ohio Data	
Di(2-ethylhexyl) sodium sulfosuccinate	577-11-7	4	10%	Suspension	n.p.		6.54	12	0.00	Severe															Hagino et al. (1999) Submitted Y. Ohio Data	
Di(2-ethylhexyl) sodium sulfosuccinate	577-11-7	5	10%	Suspension	n.p.		6.54	5	0.00	Moderate															Hagino et al. (1999) Submitted Y. Ohio Data	
Disopropanolamine	110-97-4	1	10%	Solution	n.p.		11.89	8.25	2.36	Moderate	Moderate														Hagino et al. (1999) Submitted Y. Ohio Data	
Disopropanolamine	110-97-4	2	10%	Solution	n.p.		11.89	8.5	4.04	Moderate															Hagino et al. (1999) Submitted Y. Ohio Data	
Disopropanolamine	110-97-4	3	10%	Solution	n.p.		11.89	9	1.15	Severe															Hagino et al. (1999) Submitted Y. Ohio Data	
Disopropanolamine	110-97-4	4	10%	Solution	n.p.		11.89	12	0.00	Severe															Hagino et al. (1999) Submitted Y. Ohio Data	
Disopropanolamine	110-97-4	5	10%	Solution	n.p.		11.89	5	0.00	Moderate															Hagino et al. (1999) Submitted Y. Ohio Data	

Substance Name	CASRN	Lab	In Vitro Conc. Tested	In Vitro Physical Form Tested	Purity (%)	Solubility ^a	pH	IS(A) ^b	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B) ^b	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score ^c	S-Score ^d Classification	Overall S-Score Classification	Q-Score ^e	Q-Score ^f Classification	Overall Q-Score Classification	IS(B)-10 ^g	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-10 ^h	IS(B)-10 Class.	Overall IS(B)-100 Class.	Reference
Domiphen bromide	538-71-6	1	10%	Solution	n.p.		6.22	19	0.00	Severe	Severe															Hagino et al. (1999) Submitted Y. Ohno Data		
Domiphen bromide	538-71-6	2	10%	Solution	n.p.		6.22	15.25	2.36	Severe																Hagino et al. (1999) Submitted Y. Ohno Data		
Domiphen bromide	538-71-6	3	10%	Solution	n.p.		6.22	14.75	1.50	Severe																Hagino et al. (1999) Submitted Y. Ohno Data		
Domiphen bromide	538-71-6	4	10%	Solution	n.p.		6.22	12.25	2.36	Severe																Hagino et al. (1999) Submitted Y. Ohno Data		
Domiphen bromide	538-71-6	5	10%	Solution	n.p.		6.22	9	1.22	Severe																Hagino et al. (1999) Submitted Y. Ohno Data		
Ethanol	64-17-5	1	10%	Solution	n.p.		5.9	0	0.00	Nonirritant	Slight															Hagino et al. (1999) Submitted Y. Ohno Data		
Ethanol	64-17-5	2	10%	Solution	n.p.		5.9	1.25	2.50	Slight																Hagino et al. (1999) Submitted Y. Ohno Data		
Ethanol	64-17-5	3	10%	Solution	n.p.		5.9	10.5	1.91	Severe																Hagino et al. (1999) Submitted Y. Ohno Data		
Ethanol	64-17-5	4	10%	Solution	n.p.		5.9	1.5	1.73	Slight																Hagino et al. (1999) Submitted Y. Ohno Data		
Ethanol	64-17-5	5	10%	Solution	n.p.		5.9	1.25	2.50	Slight																Hagino et al. (1999) Submitted Y. Ohno Data		
Ethanol	64-17-5	1	100%	Liquid	n.p.		18.75	3.30	Severe	Severe															Hagino et al. (1999) Submitted Y. Ohno Data			
Ethanol	64-17-5	2	100%	Liquid	n.p.		16	2.45	Severe																Hagino et al. (1999) Submitted Y. Ohno Data			
Ethanol	64-17-5	3	100%	Liquid	n.p.		11.5	1.00	Severe																Hagino et al. (1999) Submitted Y. Ohno Data			
Ethanol	64-17-5	4	100%	Liquid	n.p.		17	0.00	Severe																Hagino et al. (1999) Submitted Y. Ohno Data			
Ethanol	64-17-5	5	100%	Liquid	n.p.		10.5	1.73	Severe																Hagino et al. (1999) Submitted Y. Ohno Data			
Glycolic acid	79-14-1	1	10%	Solution	n.p.		1.76	19.5	1.00	Severe	Severe															Hagino et al. (1999) Submitted Y. Ohno Data		
Glycolic acid	79-14-1	2	10%	Solution	n.p.		1.76	20	1.15	Severe																Hagino et al. (1999) Submitted Y. Ohno Data		
Glycolic acid	79-14-1	3	10%	Solution	n.p.		1.76	17.75	3.95	Severe																Hagino et al. (1999) Submitted Y. Ohno Data		
Glycolic acid	79-14-1	4	10%	Solution	n.p.		1.76	12.25	2.36	Severe																Hagino et al. (1999) Submitted Y. Ohno Data		
Glycolic acid	79-14-1	5	10%	Solution	n.p.		1.76	12.75	2.50	Severe																Hagino et al. (1999) Submitted Y. Ohno Data		

Substance Name	CASRN	Lab	In Vitro Conc. Tested	In Vitro Physical Form Tested	Purity (%)	Solubility ^a	pH	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B) ^b	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score ^c	Overall S-Score Classification	Q-Score ^d	Q-Score Classification	Overall Q-Score Classification	IS(B)-10 ^e	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100 ^f	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Lactic acid	50-21-5	1	10%	Solution	n.p.		1.94	20.5	1.00	Severe	Severe														Hagino et al. (1999) Submitted Y. Ohno Data	
Lactic acid	50-21-5	2	10%	Solution	n.p.		1.94	14.25	2.06	Severe															Hagino et al. (1999) Submitted Y. Ohno Data	
Lactic acid	50-21-5	3	10%	Solution	n.p.		1.94	19.5	1.91	Severe															Hagino et al. (1999) Submitted Y. Ohno Data	
Lactic acid	50-21-5	4	10%	Solution	n.p.		1.94	18.5	1.91	Severe															Hagino et al. (1999) Submitted Y. Ohno Data	
Lactic acid	50-21-5	5	10%	Solution	n.p.		1.94	10.25	2.50	Severe															Hagino et al. (1999) Submitted Y. Ohno Data	
Lactic acid	50-21-5	1	100%	Liquid	n.p.			21	0.00	Severe	Severe														Hagino et al. (1999) Submitted Y. Ohno Data	
Lactic acid	50-21-5	2	100%	Liquid	n.p.			6.25	2.50	Moderate															Hagino et al. (1999) Submitted Y. Ohno Data	
Lactic acid	50-21-5	3	100%	Liquid	n.p.			16	1.15	Severe															Hagino et al. (1999) Submitted Y. Ohno Data	
Lactic acid	50-21-5	4	100%	Liquid	n.p.			15.25	2.50	Severe															Hagino et al. (1999) Submitted Y. Ohno Data	
Lactic acid	50-21-5	5	100%	Liquid	n.p.			11.5	2.89	Severe															Hagino et al. (1999) Submitted Y. Ohno Data	
Monoethanolamine	141-43-5	1	10%	Solution	n.p.		12.58	12	0.00	Severe	Severe														Hagino et al. (1999) Submitted Y. Ohno Data	
Monoethanolamine	141-43-5	2	10%	Solution	n.p.		12.58	12	0.00	Severe															Hagino et al. (1999) Submitted Y. Ohno Data	
Monoethanolamine	141-43-5	3	10%	Solution	n.p.		12.58	12	0.00	Severe															Hagino et al. (1999) Submitted Y. Ohno Data	
Monoethanolamine	141-43-5	4	10%	Solution	n.p.		12.58	12	0.00	Severe															Hagino et al. (1999) Submitted Y. Ohno Data	
Monoethanolamine	141-43-5	5	10%	Solution	n.p.		12.58	12	0.00	Severe															Hagino et al. (1999) Submitted Y. Ohno Data	
Potassium laurate	10124-65-9	1	10%	Solution	n.p.		10.49	20	1.15	Severe	Severe														Hagino et al. (1999) Submitted Y. Ohno Data	
Potassium laurate	10124-65-9	2	10%	Solution	n.p.		10.49	13.25	2.50	Severe															Hagino et al. (1999) Submitted Y. Ohno Data	
Potassium laurate	10124-65-9	3	10%	Solution	n.p.		10.49	12	0.00	Severe															Hagino et al. (1999) Submitted Y. Ohno Data	
Potassium laurate	10124-65-9	4	10%	Solution	n.p.		10.49	12	0.00	Severe															Hagino et al. (1999) Submitted Y. Ohno Data	
Potassium laurate	10124-65-9	5	10%	Solution	n.p.		10.49	19.33	0.82	Severe															Hagino et al. (1999) Submitted Y. Ohno Data	

Substance Name	CASRN	Lab	In Vitro Concentration Tested	In Vitro Physical Form Tested	Purity (%)	Solubility ^a	pH	IS(A) ^b	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B) ^b	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score ^c	S-Score Classification	Overall S-Score Classification	Q-Score ^d	Q-Score Classification	Overall Q-Score Classification	IS(B)-10 ^e	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100 ^f	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference	
Stearyltrimethylammonium chloride	15461-40-2	1	10%	Solution	n.p.		4.24	16.75	2.06	Severe	Severe																Hagino et al. (1999) Submitted Y. Ohno Data		
Stearyltrimethylammonium chloride	15461-40-2	2	10%	Solution	n.p.		4.24	13	2.00	Severe																		Hagino et al. (1999) Submitted Y. Ohno Data	
Stearyltrimethylammonium chloride	15461-40-2	3	10%	Solution	n.p.		4.24	15.75	3.50	Severe																		Hagino et al. (1999) Submitted Y. Ohno Data	
Stearyltrimethylammonium chloride	15461-40-2	4	10%	Solution	n.p.		4.24	13.5	1.00	Severe																		Hagino et al. (1999) Submitted Y. Ohno Data	
Stearyltrimethylammonium chloride	15461-40-2	5	10%	Solution	n.p.		4.24	9	0.00	Severe																		Hagino et al. (1999) Submitted Y. Ohno Data	
Triethanolamine	102-71-6	1	10%	Solution	n.p.		11.26	1.5	2.38	Slight	Slight																	Hagino et al. (1999) Submitted Y. Ohno Data	
Triethanolamine	102-71-6	2	10%	Solution	n.p.		11.26	3.75	4.79	Slight																		Hagino et al. (1999) Submitted Y. Ohno Data	
Triethanolamine	102-71-6	3	10%	Solution	n.p.		11.26	11	1.15	Severe																		Hagino et al. (1999) Submitted Y. Ohno Data	
Triethanolamine	102-71-6	4	10%	Solution	n.p.		11.26	6	1.63	Moderate																		Hagino et al. (1999) Submitted Y. Ohno Data	
Triethanolamine	102-71-6	5	10%	Solution	n.p.		11.26	2.5	2.89	Slight																		Hagino et al. (1999) Submitted Y. Ohno Data	
Triethanolamine	102-71-6	1	100%	Liquid	n.p.		5	0.00	Moderate	Moderate																		Hagino et al. (1999) Submitted Y. Ohno Data	
Triethanolamine	102-71-6	2	100%	Liquid	n.p.		6.75	3.50	Moderate																			Hagino et al. (1999) Submitted Y. Ohno Data	
Triethanolamine	102-71-6	3	100%	Liquid	n.p.		11.5	1.00	Severe																			Hagino et al. (1999) Submitted Y. Ohno Data	
Triethanolamine	102-71-6	4	100%	Liquid	n.p.		12	0.00	Severe																			Hagino et al. (1999) Submitted Y. Ohno Data	
Triethanolamine	102-71-6	5	100%	Liquid	n.p.		6.75	3.50	Moderate																			Hagino et al. (1999) Submitted Y. Ohno Data	
Ethanol	64-17-5		10%	Solution	n.p.		7.2	4		Slight	Slight																		Kojima et al. (1995)
Potassium laurate	10124-65-9		10%	Solution	98		9.4	14.3		Severe	Severe																	Kojima et al. (1995)	
Sodium lauryl sulfate	151-21-3		10%	Solution	98		5.4	7.5		Moderate	Moderate																	Kojima et al. (1995)	
Stearyltrimethylammonium chloride	15461-40-2		10%	Solution	65		5.5	19.3		Severe	Severe																	Kojima et al. (1995)	
Triton X-100	9002-93-1		10%	Solution	n.p.		5.75	5		Moderate	Moderate																	Kojima et al. (1995)	
7-Acetoxyheptanal ^g		MD	100%, 10%, and ITC	-	n.p.	insoluble	n.s.													3.1	Slight	Slight	Severe	4.9	Slight	Severe	Spielmann et al. (1996)		
7-Acetoxyheptanal		WA	100%, 10%, and ITC	-	n.p.	insoluble	n.s.													0	Nonirritant			17	Severe			Spielmann et al. (1996)	
n-Acetyl-Methionine	1115-47-5	MD	100%, 10%, and ITC	-	n.p.	83	2.2													13.6	Severe	Slight	Slight	n.p.		Slight	Spielmann et al. (1996)		

Substance Name	CASRN	Lab	In Vitro Concentration	In Vitro Physical Form Tested	Purity (%)	Solubility*	pH	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B) ^j	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score ⁱ	S-Score Classification	Overall S-Score Classification	Q-Score ^j	Q-Score Classification	Overall Q-Score Classification	IS(B)-10 ⁱ	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100 ⁱ	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
n-Acetyl-Methionine	1115-47-5	WA	100%, 10%, and ITC	-	n.p.	83	2.2														6.1	Moderate	Severe	10.6	Severe	Severe	Spielmann et al. (1996)
Ambuphylline	5634-34-4	BG	100%, 10%, and ITC	-	n.p.	600	9													10.7	Severe	Severe	12.8	Severe	Severe	Spielmann et al. (1996)	
Ambuphylline	5634-34-4	MD	100%, 10%, and ITC	-	n.p.	600	9													15.8	Severe	Severe	16.9	Severe	Severe	Spielmann et al. (1996)	
4-Amino-5-methoxy-2-methylbenzenesulfonic acid	6471-78-9	AP	100%, 10%, and ITC	-	n.p.	3	1.5													14.8	Severe	Severe	14.4	Severe	Severe	Spielmann et al. (1996)	
4-Amino-5-methoxy-2-methylbenzenesulfonic acid	6471-78-9	WA	100%, 10%, and ITC	-	n.p.	3	1.5													7	Moderate	Moderate	13.6	Severe	Severe	Spielmann et al. (1996)	
4-Amino-5-methoxy-2-methylbenzenesulfonic acid	6471-78-9	BG	100%, 10%, and ITC	-	n.p.	3	1.5													7.6	Moderate	Moderate	8.5	Moderate	Moderate	Spielmann et al. (1996)	
Ammonium persulfate	7727-54-0	HO	100%, 10%, and ITC	-	n.p.	560	1.5													4.4	Slight	Slight	n.p.			Spielmann et al. (1996)	
Ammonium persulfate	7727-54-0	WA	100%, 10%, and ITC	-	n.p.	560	1.5													n.p.			n.p.			Spielmann et al. (1996)	
Anisole	100-66-3	AP	100%, 10%, and ITC	-	n.p.	insoluble	n.s.													7.3	Moderate	Moderate	19.1	Severe	Severe	Spielmann et al. (1996)	
Anisole	100-66-3	HK	100%, 10%, and ITC	-	n.p.	insoluble	n.s.													0	Nonirritant		18.5	Severe	Severe	Spielmann et al. (1996)	
B 25		BG	100%, 10%, and ITC	-	n.p.	insoluble	n.s.													0	Nonirritant	Nonirritant	0	Nonirritant	Nonirritant	Spielmann et al. (1996)	
B 25		WA	100%, 10%, and ITC	-	n.p.	insoluble	n.s.													0	Nonirritant	Nonirritant	0	Nonirritant	Nonirritant	Spielmann et al. (1996)	
n-Butanal	123-72-8	HK	100%, 10%, and ITC	-	n.p.	71	<7													1.2	Slight	Moderate	20.3	Severe	Severe	Spielmann et al. (1996)	
n-Butanal	123-72-8	HO	100%, 10%, and ITC	-	n.p.	71	<7													6.7	Moderate	Moderate	18.1	Severe	Severe	Spielmann et al. (1996)	
n-Butanol	71-36-3	BD	100%, 10%, and ITC	-	n.p.	79	7													9.6	Severe	Severe	13	Severe	Severe	Spielmann et al. (1996)	
n-Butanol	71-36-3	HK	100%, 10%, and ITC	-	n.p.	79	7													18.3	Severe	Severe	20.2	Severe	Severe	Spielmann et al. (1996)	
Butyl carbamate	592-35-8	BD	100%, 10%, and ITC	-	n.p.	1	n.s.													0	Nonirritant	Severe	11.5	Severe	Severe	Spielmann et al. (1996)	
Butyl carbamate	592-35-8	MD	100%, 10%, and ITC	-	n.p.	1	n.s.													10.9	Severe	Severe	11.6	Severe	Severe	Spielmann et al. (1996)	
Butyl carbamate	592-35-8	BG	100%, 10%, and ITC	-	n.p.	1	n.s.													9.5	Severe	Severe	14.9	Severe	Severe	Spielmann et al. (1996)	

Substance Name	CASRN	Lab	In Vitro Concentration Tested	In Vitro Physical Form Tested	Purity (%)	Solubility*	pH	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B) ^j	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score ⁱ	S-Score Classification	Overall S-Score Classification	Q-Score ^j	Q-Score Classification	Overall Q-Score Classification	IS(B)-10 ⁱ	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-10 ^j	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Caffeine sodium benzoate	8000-95-1	BD	100%, 10%, and ITC	-	n.p.	500	7														4.6	Slight		7.4	Moderate	Spielmann et al. (1996)	
Caffeine sodium benzoate	8000-95-1	WA	100%, 10%, and ITC	-	n.p.	500	7														7.9	Moderate	Moderate	17.9	Severe	Severe	
Caffeine sodium benzoate	8000-95-1	BG	100%, 10%, and ITC	-	n.p.	500	7														6.6	Moderate		14	Severe		
Caffeine sodium salicylate	8002-85-5	BG	100%, 10%, and ITC	-	n.p.	400	7														7.4	Moderate	Severe	16	Severe	Spielmann et al. (1996)	
Caffeine sodium salicylate	8002-85-5	WA	100%, 10%, and ITC	-	n.p.	400	7														9.8	Severe	Severe	18.8	Severe	Spielmann et al. (1996)	
Camphen	79-92-5	BG	100%, 10%, and ITC	-	n.p.	insoluble	7														2	Severe	Severe	4	Slight		
Camphen	79-92-5	HK	100%, 10%, and ITC	-	n.p.	insoluble	7														10	Severe		n.p.		Spielmann et al. (1996)	
Cerium-2-ethylhexanoate	24593-34-8	BG	100%, 10%, and ITC	-	n.p.		3														6.9	Moderate	Moderate	15.1	Severe	Spielmann et al. (1996)	
Cerium-2-ethylhexanoate	24593-34-8	WA	100%, 10%, and ITC	-	n.p.		3														7.9	Moderate		19.25	Severe		
1-Chloroctane-8-ol		AP	100%, 10%, and ITC	-	n.p.	insoluble	n.s.														6.8	Moderate	Moderate	18.7	Severe	Spielmann et al. (1996)	
1-Chloroctane-8-ol		MD	100%, 10%, and ITC	-	n.p.	insoluble	n.s.														4.3	Slight		14.3	Severe		
3-Cyclohexene-1-methanol	1679-51-2	BG	100%, 10%, and ITC	-	n.p.	insoluble	n.s.														10.1	Severe	Severe	18.9	Severe	Spielmann et al. (1996)	
3-Cyclohexene-1-methanol	1679-51-2	HO	100%, 10%, and ITC	-	n.p.	insoluble	n.s.														11.8	Severe		19	Severe		
DC 8		BG	100%, 10%, and ITC	-	n.p.	insoluble	n.s.														0	Nonirritant	Nonirritant	0	Nonirritant	Spielmann et al. (1996)	
DC 8		WA	100%, 10%, and ITC	-	n.p.	insoluble	n.s.														0	Nonirritant	Moderate	5	Moderate		
1,4-Dibutoxy-benzene	104-36-9	HO	100%, 10%, and ITC	-	n.p.	0.2	7														4.2	Slight	Slight	0	Nonirritant	Spielmann et al. (1996)	
1,4-Dibutoxy-benzene	104-36-9	WA	100%, 10%, and ITC	-	n.p.	0.2	7														0	Nonirritant		n.p.		Spielmann et al. (1996)	
Diepoxy 126	2386-87-0	AP	100%, 10%, and ITC	-	n.p.	insoluble	n.s.														6	Moderate	Moderate	10	Severe	Spielmann et al. (1996)	
Diepoxy 126	2386-87-0	MD	100%, 10%, and ITC	-	n.p.	insoluble	n.s.														8.6	Moderate	Moderate	15.6	Severe	Severe	
Diepoxy 126	2386-87-0	BG	100%, 10%, and ITC	-	n.p.	insoluble	n.s.														1.9	Slight		6	Moderate		

Substance Name	CASRN	Lab	In Vitro Concentration Tested	In Vitro Physical Form Tested	Purity (%)	Solubility*	pH	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B) ^j	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score ⁱ	S-Score Classification	Overall S-Score Classification	Q-Score ^j	Q-Score Classification	Overall Q-Score Classification	IS(B)-10 ⁱ	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-10 ^j	IS(B)-10 Class.	Overall IS(B)-10 Class.	Reference
2,5-Dimethylhexanediol	110-03-2	HK	100%, 10%, and ITC	-	n.p.	n.s.														9.2	Severe		16.6	Severe		Spielmann et al. (1996)	
2,5-Dimethylhexanediol	110-03-2	HO	100%, 10%, and ITC	-	n.p.	n.s.														4.1	Slight	Severe	11.1	Severe	Severe		
2,5-Dimethylhexanediol	110-03-2	BG	100%, 10%, and ITC	-	n.p.	n.s.																					
3,6-Dimethyloctanol		BG	100%, 10%, and ITC	-	n.p.	poorly soluble	7													0.3	Nonirritant	Nonirritant	4.3	Slight	Slight	Spielmann et al. (1996)	
3,6-Dimethyloctanol		BD	100%, 10%, and ITC	-	n.p.	poorly soluble	7													0	Nonirritant	Nonirritant	4.3	Slight	Slight		
4,6-Dimethyl-3-oxo-pentanenitrile	59997-51-2	AP	100%, 10%, and ITC	-	n.p.	0.6	n.s.													4.3	Slight	Moderate	6.7	Moderate	Moderate	Spielmann et al. (1996)	
4,4-Dimethyl-3-oxo-pentanenitrile	59997-51-2	WA	100%, 10%, and ITC	-	n.p.	0.6	n.s.													5.6	Moderate	Moderate	5.7	Moderate	Moderate		
1-(2,6-dimethylphenoxy)-2-propanone	53012-41-2	HK	100%, 10%, and ITC	-	n.p.	insoluble	5													18.9	Severe	Severe	19.3	Severe	Severe	Spielmann et al. (1996)	
1-(2,6-dimethylphenoxy)-2-propanone	53012-41-2	WA	100%, 10%, and ITC	-	n.p.	insoluble	5													2.6	Slight	Severe	12	Severe	Severe		
1-(2,6-dimethylphenoxy)-2-propanone	53012-41-2	BG	100%, 10%, and ITC	-	n.p.	insoluble	5													0.75	Nonirritant	Nonirritant	4.1	Slight	Slight		
Diphocars		HK	100%, 10%, and ITC	-	n.p.	soluble	n.s.													18.3	Severe	Severe	17.9	Severe	Severe	Spielmann et al. (1996)	
Diphocars		HO	100%, 10%, and ITC	-	n.p.	soluble	n.s.													11.1	Severe	Severe	12.3	Severe	Severe		
1,2-Dodecanediol	1119-87-5	AP	100%, 10%, and ITC	-	n.p.	insoluble	n.s.													12.1	Severe	Severe	2.3	Slight	Slight	Spielmann et al. (1996)	
1,2-Dodecanediol	1119-87-5	BG	100%, 10%, and ITC	-	n.p.	insoluble	n.s.													1.8	Slight	Severe	4.1	Slight	Slight		
1,2-Dodecanediol	1119-87-5	BG	100%, 10%, and ITC	-	n.p.	insoluble	n.s.													2.54	Slight	Nonirritant					
DTTPA Pentasodium salt	140-01-2	BG	100%, 10%, and ITC	-	n.p.	readily soluble	11.5													15.66	Severe	Severe	19.4	Severe	Severe	Spielmann et al. (1996)	
DTTPA Pentasodium salt	140-01-2	WA	100%, 10%, and ITC	-	n.p.	readily soluble	11.5													15.5	Severe	Severe	19.9	Severe	Severe		
Ede 140		WA	100%, 10%, and ITC	-	n.p.	insoluble	n.s.													0	Nonirritant	Severe	0	Nonirritant	Slight	Spielmann et al. (1996)	
Ede 140		BD	100%, 10%, and ITC	-	n.p.	insoluble	n.s.													3.4	Slight	Severe	4.6	Slight	Slight		
1,2-Epoxyoctane	286-62-4	MD	100%, 10%, and ITC	-	n.p.	<2.5	4.5													n.p.		Severe	n.p.			Spielmann et al. (1996)	
1,2-Epoxyoctane	286-62-4	AP	100%, 10%, and ITC	-	n.p.	<2.5	4.5													3.1	Slight	Severe	7	Moderate	Moderate		
1,2-Epoxydodecane	2855-19-8	MD	100%, 10%, and ITC	-	n.p.	insoluble	n.s.													0	Nonirritant	Severe	1.4	Slight	Moderate	Spielmann et al. (1996)	

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12-Epoxydodecane	2855-19-8	HO	100%, 10%, and ITC	-	n.p.	insoluble	n.s.													4.1	Slight	Slight	8.5	Moderate	Moderate	Spielmann et al. (1996)	
Ethiosan		AP	100%, 10%, and ITC	-	n.p.	5	8.5													3.8	Slight	Slight	n.p.			Spielmann et al. (1996)	
Ethiosan		WA	100%, 10%, and ITC	-	n.p.	5	8.5													0	Nonirritant	n.p.	n.p.			Spielmann et al. (1996)	
Ethyl butanal	97-96-1	HO	100%, 10%, and ITC	-	n.p.	10	<7													3.6	Slight	Slight	17.4	Severe	Severe	Spielmann et al. (1996)	
Ethyl butanal	97-96-1	WA	100%, 10%, and ITC	-	n.p.	10	<7													0	Nonirritant	Slight	18.7	Severe	Severe	Spielmann et al. (1996)	
Gadopentetic acid dimeglumine salt	86050-77-3	WA	100%, 10%, and ITC	-	n.p.	soluble	n.s.													6.4	Severe	Severe	8.2	Moderate	Moderate	Spielmann et al. (1996)	
Gadopentetic acid dimeglumine salt	86050-77-3	BG	100%, 10%, and ITC	-	n.p.	soluble	n.s.													3	Severe	Severe	3.2	Slight		Spielmann et al. (1996)	
Genomoll	115-96-8	HO	100%, 10%, and ITC	-	n.p.	5	6													9.2	Severe	Severe	11.6	Severe	Severe	Spielmann et al. (1996)	
Genomoll	115-96-8	WA	100%, 10%, and ITC	-	n.p.	5	6													9.4	Severe	Severe	9.9	Severe		Spielmann et al. (1996)	
C12/C14-Glucoside		BD	100%, 10%, and ITC	-	n.p.	readily soluble	9													8.4	Moderate	Severe	16.7	Severe		Spielmann et al. (1996)	
C12/C14-Glucoside		HK	100%, 10%, and ITC	-	n.p.	readily soluble	9													10.1	Severe	Severe	16.3	Severe	Severe	Spielmann et al. (1996)	
C12/C14-Glucoside		BG	100%, 10%, and ITC	-	n.p.	readily soluble	9													10.2	Severe	Severe	16.5	Severe		Spielmann et al. (1996)	
L-Glutamic acid hydrochloride	138-15-8	HO	100%, 10%, and ITC	-	n.p.	490	0.9													14.2	Severe	Severe	11.7	Severe	Severe	Spielmann et al. (1996)	
L-Glutamic acid hydrochloride	138-15-8	MD	100%, 10%, and ITC	-	n.p.	490	0.9													11.7	Severe	Severe	15.2	Severe		Spielmann et al. (1996)	
Glycidol		MD	100%, 10%, and ITC	-	n.p.	insoluble	n.s.													0	Nonirritant	Severe	0.58	Nonirritant	Slight	Spielmann et al. (1996)	
Glycidol		HO	100%, 10%, and ITC	-	n.p.	insoluble	n.s.													1.8	Slight	Severe	3.5	Slight		Spielmann et al. (1996)	
Granuforn	30525-89-4	BD	100%, 10%, and ITC	-	n.p.	250	4													2.9	Slight	Severe	0	Nonirritant	Nonirritant	Spielmann et al. (1996)	
Granuforn	30525-89-4	HO	100%, 10%, and ITC	-	n.p.	250	4													0	Nonirritant	Severe	0	Nonirritant		Spielmann et al. (1996)	
Hexahydrofarnesylacetone	502-69-2	BG	100%, 10%, and ITC	-	n.p.	poorly soluble	n.s.													2.3	Slight	Severe	8	Moderate	Moderate	Spielmann et al. (1996)	
Hexahydrofarnesylacetone	502-69-2	BD	100%, 10%, and ITC	-	n.p.	poorly soluble	n.s.													1.2	Slight	Severe	4.2	Slight		Spielmann et al. (1996)	
Hexamethylenetetramine	100-97-0	WA	100%, 10%, and ITC	-	n.p.	874	8.5													5.8	Moderate	Severe	11.1	Severe	Severe	Spielmann et al. (1996)	
Hexamethylenetetramine	100-97-0	MD	100%, 10%, and ITC	-	n.p.	874	8.5													4.3	Slight	Severe	11.2	Severe	Severe	Spielmann et al. (1996)	

Substance Name	CASRN	Lab	In Vitro Concentration Tested	In Vitro Physical Form Tested	Purity (%)	Solubility*	pH	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B) ^j	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score ⁱ	S-Score Classification	Overall S-Score Classification	Q-Score ^j	Q-Score Classification	Overall Q-Score Classification	IS(B)-10 ⁱ	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100 ⁱ	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
1,2,6-Hexanetriol	106-69-4	HK	100%, 10%, and ITC	-	n.p.		4.5														11.5	Severe	Severe	18.8	Severe	Severe	Spielmann et al. (1996)
1,2,6-Hexanetriol	106-69-4	HO	100%, 10%, and ITC	-	n.p.		4.5														4.3	Slight		15.3	Severe		Spielmann et al. (1996)
Hnol		AP	100%, 10%, and ITC	-	n.p.	insoluble	n.s.														0.8	Nonirritant	Nonirritant	2.1	Slight	Moderate	Spielmann et al. (1996)
Hnol		WA	100%, 10%, and ITC	-	n.p.	insoluble	n.s.														0	Nonirritant		6	Moderate		Spielmann et al. (1996)
Hoe MBF		BD	100%, 10%, and ITC	-	n.p.	100	4.3														0	Nonirritant	Nonirritant	0	Nonirritant	Nonirritant	Spielmann et al. (1996)
Hoe MBF		MD	100%, 10%, and ITC	-	n.p.	100	4.3														0	Nonirritant		0.35	Nonirritant		Spielmann et al. (1996)
Hydo 98		BD	100%, 10%, and ITC	-	n.p.	soluble	6.5														10.4	Severe	Severe	11.2	Severe	Severe	Spielmann et al. (1996)
Hydo 98		MD	100%, 10%, and ITC	-	n.p.	soluble	6.5														12.9	Severe		n.p.			Spielmann et al. (1996)
2-Hydroxyethyl imino disodium acetate	135-37-5	AP	100%, 10%, and ITC	-	n.p.		10.6														13.4	Severe	Severe	15.5	Severe	Severe	Spielmann et al. (1996)
2-Hydroxyethyl imino disodium acetate	135-37-5	HO	100%, 10%, and ITC	-	n.p.		10.6														8.9	Moderate		11	Severe		Spielmann et al. (1996)
2-Hydroxyisobutyric acid	594-61-6	BD	100%, 10%, and ITC	-	n.p.	1900	1														10.8	Severe	Severe	11.3	Severe	Severe	Spielmann et al. (1996)
2-Hydroxyisobutyric acid	594-61-6	WA	100%, 10%, and ITC	-	n.p.	1900	1														14.9	Severe		15.6	Severe		Spielmann et al. (1996)
Hypo 20		BG	100%, 10%, and ITC	-	n.p.	readily soluble	6.5														7.2	Moderate	Moderate	8.9	Moderate	Moderate	Spielmann et al. (1996)
Hypo 20		HO	100%, 10%, and ITC	-	n.p.	readily soluble	6.5														0	Nonirritant		4.12	Slight		Spielmann et al. (1996)
Hypo 36		AP	100%, 10%, and ITC	-	n.p.	readily soluble	7														4	Severe	Severe	15.9	Severe	Severe	Spielmann et al. (1996)
Hypo 36		WA	100%, 10%, and ITC	-	n.p.	readily soluble	7														4.2	Severe		10	Severe		Spielmann et al. (1996)
Hypo 45		BD	100%, 10%, and ITC	-	n.p.	readily soluble	7														11.1	Severe	Slight	4.4	Slight	Severe	Spielmann et al. (1996)
Hypo 45		WA	100%, 10%, and ITC	-	n.p.	readily soluble	7														2.5	Slight		8.7	Moderate		Spielmann et al. (1996)
Hypo 45		BG	100%, 10%, and ITC	-	n.p.	readily soluble	7														1.9	Slight		11.9	Severe		Spielmann et al. (1996)
Hypo 54		BG	100%, 10%, and ITC	-	n.p.	soluble	6.5														4.3	Slight	Slight	4.1	Slight	Slight	Spielmann et al. (1996)
Hypo 54		HO	100%, 10%, and ITC	-	n.p.	soluble	6.5														4	Slight		4.2	Slight		Spielmann et al. (1996)
Hyton		AP	100%, 10%, and ITC	-	n.p.	soluble	8.5														17	Severe	Slight	18.6	Severe	Slight	Spielmann et al. (1996)

Substance Name	CASRN	Lab	In Vitro Concentration Tested	In Vitro Physical Form Tested	Purity (%)	Solubility*	pH	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B) ^j	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score ⁱ	S-Score Classification	Overall S-Score Classification	Q-Score ⁱ	Q-Score Classification	Overall Q-Score Classification	IS(B)-10 ^j	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100 ^j	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Hyton		BG	100%, 10%, and ITC	-	n.p.	soluble	8.5														13.5	Severe	Severe	18.2	Severe	Severe	Spielmann et al. (1996)
Iminodiacetic acid	142-73-4	AP	100%, 10%, and ITC	-	n.p.	42	2.3														15.6	Severe		12.8	Severe		Spielmann et al. (1996)
Iminodiacetic acid	142-73-4	BD	100%, 10%, and ITC	-	n.p.	42	2.3														0.75	Nonirritant	Severe	0.85	Nonirritant	Severe	Spielmann et al. (1996)
Iminodiacetic acid	142-73-4	BG	100%, 10%, and ITC	-	n.p.	42	2.3														8.4	Moderate		6.9	Moderate		Spielmann et al. (1996)
Isobornyl acetate	125-12-2	HO	100%, 10%, and ITC	-	n.p.	<1	n.s.														4.1	Slight		4.6	Slight		Spielmann et al. (1996)
Isobornyl acetate	125-12-2	BD	100%, 10%, and ITC	-	n.p.	<1	n.s.														1.7	Slight		8.1	Moderate		Spielmann et al. (1996)
Isobutanal	78-84-2	WA	100%, 10%, and ITC	-	n.p.	67	<7														2.1	Slight		19.4	Severe		Spielmann et al. (1996)
Isobutanal	78-84-2	HK	100%, 10%, and ITC	-	n.p.	67	<7														0	Nonirritant		20	Severe		Spielmann et al. (1996)
Iododecylglucoside		AP	100%, 10%, and ITC	-	n.p.	readily soluble	9														17.2	Severe		18	Severe		Spielmann et al. (1996)
Iododecylglucoside		HO	100%, 10%, and ITC	-	n.p.	readily soluble	9														9.9	Severe		10.7	Severe		Spielmann et al. (1996)
Isononylaldehyde	35127-50-5	BG	100%, 10%, and ITC	-	n.p.	0.1	<7														0	Nonirritant		4.5	Slight		Spielmann et al. (1996)
Isononylaldehyde	35127-50-5	WA	100%, 10%, and ITC	-	n.p.	0.1	<7														0	Nonirritant		10	Severe		Spielmann et al. (1996)
alpha-Ketoglutaric acid	328-50-7	AP	100%, 10%, and ITC	-	n.p.	1000	1.75														19.1	Severe		19.8	Severe		Spielmann et al. (1996)
alpha-Ketoglutaric acid	328-50-7	BG	100%, 10%, and ITC	-	n.p.	1000	1.75														18.8	Severe		19.7	Severe		Spielmann et al. (1996)
Lactic acid	79-33-4	Phl	100%, 10%, and ITC	-	n.p.	readily soluble	2														17.6	Severe	Severe	19.6	Severe	Severe	Spielmann et al. (1996)
alpha-Lactid	4511-42-6	AP	100%, 10%, and ITC	-	n.p.	soluble	3														13.5	Severe		4	Slight		Spielmann et al. (1996)
alpha-Lactid	4511-42-6	BG	100%, 10%, and ITC	-	n.p.	soluble	3														1.8	Slight		1.1	Slight		Spielmann et al. (1996)
alpha-Lactid	4511-42-6	BG	100%, 10%, and ITC	-	n.p.	soluble	3														10.5	Severe		6.6	Moderate		Spielmann et al. (1996)
L-Lysine Monohydrate	39665-12-8	BD	100%, 10%, and ITC	-	n.p.	1500	10														10	Severe		10.4	Severe		Spielmann et al. (1996)
L-Lysine Monohydrate	39665-12-8	HO	100%, 10%, and ITC	-	n.p.	1500	10														8.25	Moderate		16.9	Severe		Spielmann et al. (1996)
Meere		HK	100%, 10%, and ITC	-	n.p.	mixable	7														n.p.			n.p.			Spielmann et al. (1996)
Meere		MD	100%, 10%, and ITC	-	n.p.	mixable	7														n.p.			n.p.			Spielmann et al. (1996)
3-Mercapto-1,2,4-triazole	3179-31-5	HK	100%, 10%, and ITC	-	n.p.	85	4														18.3	Severe		n.p.			Spielmann et al. (1996)
3-Mercapto-1,2,4-triazole	3179-31-5	MD	100%, 10%, and ITC	-	n.p.	85	4														4.3	Slight		n.p.			Spielmann et al. (1996)
m-Methoxybenzaldehyde	591-31-1	MD	100%, 10%, and ITC	-	n.p.	poorly soluble	n.s.														4.1	Slight		13.7	Severe		Spielmann et al. (1996)
m-Methoxybenzaldehyde	591-31-1	BD	100%, 10%, and ITC	-	n.p.	poorly soluble	n.s.													2.2	Slight		11.6	Severe		Spielmann et al. (1996)	

Substance Name	CASRN	Lab	<i>In Vitro</i> Conc. Tested	<i>In Vitro</i> Physical Form Tested	Purity (%)	Solubility ^a	pH	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S- Score ^c	S-Score ^c	Overall S-Score ^c	Q- Score ^d	Q-Score ^d	Overall Q- Score ^d	IS(B)-10 ^e	IS(B)-10 ^e	Overall IS(B)- 10 Class.	IS(B)-10 ^f	IS(B)-10 ^f	Overall IS(B)-100 Class.	Reference
Methyl acetate	79-20-9	BD	100%, 10%, and ITC	-	n.p.	250	7													4.4	Slight		19.8	Severe	Severe Spielmann et al. (1996)	
Methyl acetate	79-20-9	HO	100%, 10%, and ITC	-	n.p.	250	7													4.3	Slight		16.1	Severe		
Methylpentynol	77-75-8	AP	100%, 10%, and ITC	-	n.p.	soluble	n.s.													15.4	Severe		20.1	Severe	Severe Spielmann et al. (1996)	
Methylpentynol	77-75-8	BD	100%, 10%, and ITC	-	n.p.	soluble	n.s.													12.3	Severe		12.9	Severe		
N-(2-methylphenyl)-Imidodi- carbonimidic diamide	93-69-6	AP	100%, 10%, and ITC	-	n.p.	40	11.5													17.1	Severe		4.7	Slight	Slight Spielmann et al. (1996)	
N-(2-methylphenyl)-Imidodi- carbonimidic diamide	93-69-6	MD	100%, 10%, and ITC	-	n.p.	40	11.5													17.7	Severe		n.p.			
2-Methyl-1-propanol	78-83-1	HK	100%, 10%, and ITC	-	n.p.	15	3													17.7	Severe		20.4	Severe	Severe Spielmann et al. (1996)	
2-Methyl-1-propanol	78-83-1	MD	100%, 10%, and ITC	-	n.p.	15	3													17.9	Severe		19.2	Severe		
Methyltriglycol	112-35-6	BD	100%, 10%, and ITC	-	n.p.	readily soluble	7													4.9	Slight		12.5	Severe	Severe Spielmann et al. (1996)	
Methyltriglycol	112-35-6	HO	100%, 10%, and ITC	-	n.p.	readily soluble	7													4.1	Severe		17	Severe		
Methyltriglycol	112-35-6	AP	100%, 10%, and ITC	-	n.p.	readily soluble	7													11	Severe		20.4	Severe	Severe Spielmann et al. (1996)	
Methyltriglycol	112-35-6	HO	100%, 10%, and ITC	-	n.p.	readily soluble	7													3	Severe		12.8	Severe		
Napt		HO	100%, 10%, and ITC	-	n.p.	1000	n.s.													4.3	Slight		10.3	Severe	Severe Spielmann et al. (1996)	
Napt		WA	100%, 10%, and ITC	-	n.p.	1000	n.s.													1.9	Slight		5.7	Moderate		
Nitro-bis-octylamide		BG	100%, 10%, and ITC	-	n.p.	insoluble	n.s.													1.7	Slight		6.5	Moderate	Moderate Spielmann et al. (1996)	
Nitro-bis-octylamide		HK	100%, 10%, and ITC	-	n.p.	insoluble	n.s.													0	Nonirritant		1.6	Slight		
OlaK		HK	100%, 10%, and ITC	-	n.p.	soluble	8.3													18.9	Severe		19.5	Severe	Severe Spielmann et al. (1996)	
OlaK		MD	100%, 10%, and ITC	-	n.p.	soluble	8.3													16.1	Severe		17	Severe		
Ötesulf		BD	100%, 10%, and ITC	-	n.p.	soluble	8													16.9	Severe		18.9	Severe	Severe Spielmann et al. (1996)	
Ötesulf		HK	100%, 10%, and ITC	-	n.p.	soluble	8													16.8	Severe		19.6	Severe		
Phenylephrine hydrochloride	61-76-7	AP	100%, 10%, and ITC	-	n.p.	1000	7													8.6	Moderate		18.3	Severe	Severe Spielmann et al. (1996)	
Phenylephrine hydrochloride	61-76-7	HK	100%, 10%, and ITC	-	n.p.	1000	7													11.1	Severe		19.9	Severe		

Substance Name	CASRN	Lab	In Vitro Conc. Tested	In Vitro Physical Form Tested	Purity (%)	Solubility ^a	pH	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B) ^j	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score ⁱ	S-Score Classification	Overall S-Score Classification	Q-Score ^k	Q-Score Classification	Overall Q-Score Classification	IS(B)-10 ^l	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100 ^m	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Phenylthiourea	103-85-5	AP	100%, 10% and ITC	-	n.p.	1	5.5													4	Slight		3.1	Slight		Spielmann et al. (1996)	
Phenylthiourea	103-85-5	BD	100%, 10% and ITC	-	n.p.	1	5.5													0	Nonirritant		0	Nonirritant		Spielmann et al. (1996)	
Phosphonat A		AP	100%, 10% and ITC	-	n.p.	3.6	2.1													6.8	Moderate		3.5	Slight		Spielmann et al. (1996)	
Phosphonat A		BG	100%, 10% and ITC	-	n.p.	3.6	2.1													6.6	Moderate		10.1	Severe		Spielmann et al. (1996)	
Acefyllin piperazine	18833-13-1	HK	100%, 10% and ITC	-	n.p.	625	5													18.5	Severe		15.3	Severe		Spielmann et al. (1996)	
Acefyllin piperazine	18833-13-1	WA	100%, 10% and ITC	-	n.p.	625	5													0	Nonirritant		14.6	Severe		Spielmann et al. (1996)	
Acefyllin piperazine	18833-13-1	BG	100%, 10% and ITC	-	n.p.	625	5													2.9	Slight		9	Severe		Spielmann et al. (1996)	
PO 2		AP	100%, 10% and ITC	-	n.p.	insoluble	n.s.													4.3	Slight		0.3	Nonirritant		Spielmann et al. (1996)	
PO 2		WA	100%, 10% and ITC	-	n.p.	insoluble	n.s.													0	Nonirritant		0	Nonirritant		Spielmann et al. (1996)	
Polyethylene glycol butyl ether	9004-77-7	AP	100%, 10% and ITC	-	n.p.	1000	6													10.9	Severe		19.3	Severe		Spielmann et al. (1996)	
Polyethylene glycol butyl ether	9004-77-7	WA	100%, 10% and ITC	-	n.p.	1000	6													15.7	Severe		19.2	Severe		Spielmann et al. (1996)	
Polyethylene glycol dimethyl ether	24991-55-7	HO	100%, 10% and ITC	-	n.p.	readily soluble	7													4.1	Slight		7.6	Moderate		Spielmann et al. (1996)	
Polyethylene glycol dimethyl ether	24991-55-7	WA	100%, 10% and ITC	-	n.p.	readily soluble	7													0	Nonirritant		19.8	Severe		Spielmann et al. (1996)	
Polyethylene glycol	25322-68-3	MD	100%, 10% and ITC	-	n.p.	750	n.s.													1	Slight		6.6	Moderate		Spielmann et al. (1996)	
Polyethylene glycol	25322-68-3	WA	100%, 10% and ITC	-	n.p.	750	n.s.													0	Nonirritant		7.7	Moderate		Spielmann et al. (1996)	
Polyhexamethylene guanidine		BD	100%, 10% and ITC	-	n.p.	soluble	7.1													9.2	Severe		15.5	Severe		Spielmann et al. (1996)	
Polyhexamethylene guanidine		BG	100%, 10% and ITC	-	n.p.	soluble	7.1													11	Severe		14.6	Severe		Spielmann et al. (1996)	
Polysolvan	7397-62-8	AP	100%, 10% and ITC	-	n.p.	80	7													16.5	Severe		19.4	Severe		Spielmann et al. (1996)	
Polysolvan	7397-62-8	HO	100%, 10% and ITC	-	n.p.	80	7													15.8	Severe		15.9	Severe		Spielmann et al. (1996)	
Potassium cyanate	590-28-3	AP	100%, 10% and ITC	-	n.p.	750	10													18.8	Severe		19.4	Severe		Spielmann et al. (1996)	
Potassium cyanate	590-28-3	MD	100%, 10% and ITC	-	n.p.	750	10													15.9	Severe		15.9	Severe		Spielmann et al. (1996)	
Potassium hexacyanoferrate II	14459-95-1	HK	100%, 10% and ITC	-	n.p.	250	9.5													17.8	Severe		17.2	Severe		Spielmann et al. (1996)	
Potassium hexacyanoferrate II	14459-95-1	HO	100%, 10% and ITC	-	n.p.	250	9.5													15.2	Severe		6.3	Moderate		Spielmann et al. (1996)	
Potassium hexacyanoferrate III	13756-66-2	BD	100%, 10% and ITC	-	n.p.	310	8													4.2	Slight		5.7	Moderate		Spielmann et al. (1996)	
Potassium hexacyanoferrate III	13756-66-2	MD	100%, 10% and ITC	-	n.p.	310	8													6.25	Moderate		6.45	Moderate		Spielmann et al. (1996)	
2-Pseudojonon		HK	100%, 10% and ITC	-	n.p.	0.1	n.s.													8.7	Moderate		7.3	Moderate		Spielmann et al. (1996)	
2-Pseudojonon		BG	100%, 10% and ITC	-	n.p.	0.1	n.s.													2.8	Slight		4.1	Slight		Spielmann et al. (1996)	

Substance Name	CASRN	Lab	<i>In Vitro</i> Conc. Tested	<i>In Vitro</i> Physical Form Tested	Purity (%)	Solubility*	pH	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S- Score [†]	S-Score [‡]	Overall S-Score [‡]	Q- Score [†]	Q-Score [‡]	Overall Q- Score [‡]	IS(B)-10 [§]	IS(B)-10 Class.	Overall IS(B)- 10 Class.	IS(B)-10 [¶]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
RK Blau		HK	100%, 10% and ITC	-	n.p.	100	2.6													4	Slight		n.p.		Spielmann et al. (1996)	
RK Blau		MD	100%, 10% and ITC	-	n.p.	100	2.6													0	Nonirritant		n.p.			
Rubinrot Y		AP	100%, 10% and ITC	-	n.p.	172														n.p.			5.3	Moderate	Spielmann et al. (1996)	
Rubinrot Y		HO	100%, 10% and ITC	-	n.p.	172														4	Slight		n.p.			
Sacyclo		HO	100%, 10% and ITC	-	n.p.	insoluble	n.s.													3.4	Slight		4.4	Slight	Spielmann et al. (1996)	
Sacyclo		MD	100%, 10% and ITC	-	n.p.	insoluble	n.s.													0	Nonirritant		3.3	Slight		
Sept		BD	100%, 10% and ITC	-	n.p.	soluble	3													4	Severe		15.9	Severe	Spielmann et al. (1996)	
Sept		HK	100%, 10% and ITC	-	n.p.	soluble	3													10	Severe		19.8	Severe		
Trimethoxypropylsilane	1067-25-0	BD	100%, 10% and ITC	-	n.p.	poorly soluble	n.s.													3.7	Slight		4.5	Slight	Spielmann et al. (1996)	
Trimethoxypropylsilane	1067-25-0	AP	100%, 10% and ITC	-	n.p.	poorly soluble	n.s.													3.9	Slight		13.7	Severe		
Trimethoxyoctylsilane	3069-40-7	HO	100%, 10% and ITC	-	n.p.	insoluble	n.s.													7.9	Moderate		8.4	Moderate	Spielmann et al. (1996)	
Trimethoxyoctylsilane	3069-40-7	BG	100%, 10% and ITC	-	n.p.	insoluble	n.s.													2.1	Slight		10	Severe		
Silan 165	29055-11-6	HO	100%, 10% and ITC	-	n.p.	insoluble	n.s.													0.7	Nonirritant		4.1	Slight	Spielmann et al. (1996)	
Silan 165	29055-11-6	WA	100%, 10% and ITC	-	n.p.	insoluble	n.s.													0	Nonirritant		7.2	Moderate		
Silan 167	41453-78-5	WA	100%, 10% and ITC	-	n.p.	soluble	n.s.													2.7	Slight		4.7	Slight	Spielmann et al. (1996)	
Silan 167	41453-78-5	HO	100%, 10% and ITC	-	n.p.	soluble	n.s.													0.1	Nonirritant		2.3	Slight		
Silan 253	18784-74-2	BD	100%, 10% and ITC	-	n.p.	insoluble	<7													3	Severe		9.9	Severe	Spielmann et al. (1996)	
Silan 253	18784-74-2	MD	100%, 10% and ITC	-	n.p.	insoluble	<7													3	Severe		14.7	Severe		
Sodium bisulfite	7631-90-5	AP	100%, 10% and ITC	-	n.p.	readily soluble	4.5													12.7	Severe		20	Severe	Spielmann et al. (1996)	
Sodium bisulfite	7631-90-5	MD	100%, 10% and ITC	-	n.p.	readily soluble	4.5													13.9	Severe		16.8	Severe		
Sodium sulfite	7757-83-7	AP	100%, 10% and ITC	-	n.p.	250	10													13.2	Severe		16.1	Severe	Spielmann et al. (1996)	
Sodium sulfite	7757-83-7	BG	100%, 10% and ITC	-	n.p.	250	10													11.3	Severe		12.3	Severe		
Sodium cyanate	917-61-3	MD	100%, 10% and ITC	-	n.p.	110	10.4													14.8	Severe		8.2	Moderate	Spielmann et al. (1996)	
Sodium cyanate	917-61-3	WA	100%, 10% and ITC	-	n.p.	110	10.4													10.5	Severe		10.7	Severe		
Sodium disilicate	13870-28-5	BG	100%, 10% and ITC	-	n.p.	3.5	11.4													19.7	Severe		18.2	Severe	Spielmann et al. (1996)	
Sodium disilicate	13870-28-5	HK	100%, 10% and ITC	-	n.p.	3.5	11.4													20.7	Severe		16.6	Severe		

Substance Name	CASRN	Lab	In Vitro Conc. Tested	In Vitro Physical Form Tested	Purity (%)	Solubility*	pH	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B) ^j	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score ⁱ	S-Score Classification	Overall S-Score Classification	Q-Score ⁱ	Q-Score Classification	Overall Q-Score Classification	IS(B)-10 ^j	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-10 ^j	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Sodium hydrogen sulfate	7681-38-1	HK	100%, 10% and ITC	-	n.p.	1080	1.1													18.8	Severe		19.2	Severe	Spielmann et al. (1996)		
Sodium hydrogen sulfate	7681-38-1	WA	100%, 10% and ITC	-	n.p.	1080	1.1													16.7	Severe		18.1	Severe			
Sodium lauryl ether sulfate	3088-31-1	BG	100%, 10% and ITC	-	n.p.	soluble	8													10.5	Severe		17.9	Severe	Spielmann et al. (1996)		
Sodium lauryl ether sulfate	3088-31-1	MD	100%, 10% and ITC	-	n.p.	soluble	8													17.7	Severe		19	Severe			
Sodium monochloroacetate	3926-62-3	HO	100%, 10% and ITC	-	n.p.	440	4.5													7.5	Moderate		16.1	Severe	Spielmann et al. (1996)		
Sodium monochloroacetate	3926-62-3	BD	100%, 10% and ITC	-	n.p.	440	4.5													0	Nonirritant		10.8	Severe			
Sodium pyrosulfite	7681-57-4	AP	100%, 10% and ITC	-	n.p.	650	4.6													17.4	Severe		17.7	Severe	Spielmann et al. (1996)		
Sodium pyrosulfite	7681-57-4	BD	100%, 10% and ITC	-	n.p.	650	4.6													12.6	Severe		11.6	Severe			
Sodium pyrosulfite	7681-57-4	BG	100%, 10% and ITC	-	n.p.	650	4.6													14.6	Severe		14.5	Severe	Spielmann et al. (1996)		
4-(2-sulfatoethyl)sulfonyl-aniline	2494-89-5	AP	100%, 10% and ITC	-	n.p.	soluble	7													18	Severe		10.4	Severe			
4-(2-sulfatoethyl)sulfonyl-aniline	2494-89-5	HK	100%, 10% and ITC	-	n.p.	soluble	7													20.1	Severe		n.p.	Severe	Spielmann et al. (1996)		
TA 01946 Alkylsilan		AP	100%, 10% and ITC	-	n.p.	0.014	n.s.													7.6	Moderate		16.2	Severe	Spielmann et al. (1996)		
TA 01946 Alkylsilan		HK	100%, 10% and ITC	-	n.p.	0.014	n.s.													10	Severe		10	Severe			
Theophylline sodium acetate	8002-89-9	AP	100%, 10% and ITC	-	n.p.	50	11													13.4	Severe		6.9	Moderate	Spielmann et al. (1996)		
Theophylline sodium acetate	8002-89-9	HO	100%, 10% and ITC	-	n.p.	50	11													5.4	Moderate		n.p.	Severe			
Tocla		BD	100%, 10% and ITC	-	n.p.	40	6													12.9	Severe		13.5	Severe	Spielmann et al. (1996)		
Tocla		HK	100%, 10% and ITC	-	n.p.	40	6													19.7	Severe		20.4	Severe			
Trisooctylamine	25549-16-0	BG	100%, 10% and ITC	-	n.p.	0.5	7													0.8	Nonirritant		14.1	Severe	Spielmann et al. (1996)		
Trisooctylamine	25549-16-0	MD	100%, 10% and ITC	-	n.p.	0.5	7													0	Nonirritant		4	Slight			
2,2,3-Trimethyl-3-Cyclopentene-1-acetaldehyde	4501-58-0	BG	100%, 10% and ITC	-	n.p.	< 2.5	2.3													2.9	Slight		9.7	Severe	Spielmann et al. (1996)		
2,2,3-Trimethyl-3-Cyclopentene-1-acetaldehyde	4501-58-0	AP	100%, 10% and ITC	-	n.p.	< 2.5	2.3													2.3	Slight		14.7	Severe			
Trioxane	110-88-3	HK	100%, 10% and ITC	-	n.p.	172	n.s.													9.25	Severe		18	Severe	Spielmann et al. (1996)		
Trioxane	110-88-3	WA	100%, 10% and ITC	-	n.p.	172	n.s.													13.4	Severe		17.8	Severe			
Wessalith Slurry		BG	100%, 10% and ITC	-	n.p.	readily soluble	11													3.13	Slight		4.1	Slight	Spielmann et al. (1996)		
Wessalith Slurry		WA	100%, 10% and ITC	-	n.p.	readily soluble	11													10	Severe		15.7	Severe			
Xanthinol nicotinate	437-74-1	WA	100%, 10% and ITC	-	n.p.	250	6													4	Slight		9	Severe	Spielmann et al. (1996)		
Xanthinol nicotinate	437-74-1	HK	100%, 10% and ITC	-	n.p.	250	6													11.3	Severe		17.4	Severe			

Substance Name	CASRN	Lab	<i>In Vitro</i> Conc. Tested	<i>In Vitro</i> Physical Form Tested	Purity (%)	Solubility*	pH	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B) [†]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score [‡]	S-Score Classification	Overall S-Score Classification	Q-Score [§]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10 [¶]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100 [¶]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Sodium lauryl sulfate	151-21-3		1%	Solution	n.p.		3.3				14.22		Severe													Vinardell and Macián (1994)	
Tween 20	9005-64-5		100%	Liquid	n.p.		7.21				3.22		Slight													Vinardell and Macián (1994)	

Abbreviations: CASRN = Chemical Abstract Service Registry Number, n.a. = not applicable, n.p. = not provided, Conc. = Concentration, IS = Irritation Score, ITC = Irritation Threshold Concentration, SD = standard deviation.

* Solubility = obtained from literature references; where available, expressed as g/ml.

[†] IS(A) represents irritation scores that were calculated using the method described in Leupke (1985)

[‡] IS(B) represents irritation scores that were calculated using a method similar to the one described in Kalweit et al. (1987, 1990)

[§] S-Score represents irritation scores that were calculated using the method described in Balls et al. (1995)

[¶] Q-Score represents irritation scores that were calculated using the method described in Balls et al. (1995)

[¶] IS(B)-10 and IS(B)-100 represents irritation scores that were calculated using a method similar to the one described in Kalweit et al. (1987, 1990) where the *in vitro* score was obtained using a 10% or 100% concentration, respectively.

[¶] The IS(B) analysis method does not yield an IS value greater than 21 and the calculated result of 23 for this substance is not possible. Based on results with the IS(A) analysis method (IS(A) = 17.8), the formulation would be classified as a severe irritant and was classified as such for the IS(B) analysis method.

[¶] No information on the *in vitro* physical form of substances tested by Spielmann et al. (1996) were added since the tested form depended on the concentration being evaluated (10% or 100%). For information on the tested form *in vivo* see Appendix D.